CONSTRUCTION OF HADAMARD STATES BY PSEUDO-DIFFERENTIAL CALCULUS

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Abstract. We give a new construction based on pseudo-differential calculus of quasi-free Hadamard states for Klein-Gordon equations on a class of space-times whose metric is well-behaved at spatial infinity. In particular we construct all pure Hadamard states and study their covariance under symplectic transformations. Using our results we give a new construction of Hadamard states on arbitrary globally hyperbolic space-times.

1. Introduction

1.1. **Hadamard states.** Hadamard states are nowadays widely accepted as possible physical states of the non-interacting quantum field theory on a curved space-time. One of the main reason is their applicability to renormalization of the stress-energy tensor, a necessary step in the formulation of semi-classical Einstein equations. Moreover, the Hadamard condition plays an essential role in the perturbative construction of interacting quantum field theory [BF]. Other related concepts making use of Hadamard states include local thermal equilibrium [SV] and quantum energy inequalities [FV].

Since the work of Radzikowski [R], the Hadamard condition (renamed *microlocal spectrum condition*), is formulated as a requirement for the wave front set of the associated two-point function Λ, which is necessarily a bi-solution of the free equations of motion. It is therefore natural to try to construct such states using the standard apparatus of microlocal analysis, based on pseudo-differential calculus. Although a construction is already known for space-times with compact Cauchy surface [J1], it does certainly not cover many cases of physical interest and lacks the capability to produce many states on a fixed space-time with distinct properties.

In this paper we address these questions in all generality and construct on an arbitrary globally hyperbolic space-time large classes of Hadamard states for the Klein-Gordon equation, allowing also for external potentials. We obtain complete and transparent results for space-times whose metric components are suitably well-behaved at spatial infinity. Namely, we construct in this case *all* pure quasi-free Hadamard states, whose 'symplectically smeared' two-point function λ is the integral kernel of pseudo-differential operators.

1.2. **Methods.** Our analysis is set on three levels:

(1) Our starting point are normally hyperbolic operators on $\mathbb{R}\times\mathbb{R}^d$ of the form

$$\partial_t^2 + a(t,\mathrm{x},D_{\mathrm{x}}) = \partial_t^2 - \partial_{\mathrm{x}^j} a^{jk}\partial_{\mathrm{x}^k} + b^j\partial_{\mathrm{x}^j} - \partial_{\mathrm{x}^j}\overline{b}^j + m, \tag{1.1}$$

where

$$\begin{aligned} &a^{jk}, b^j, m \in C^\infty(\mathbb{R}, C^\infty_{\rm bd}(\mathbb{R}^d)),\ m(x)\in\mathbb{R},\\ &[a^{jk}](x) \geq c(t)\mathbb{1} \ \text{ uniformly on } \mathbb{R}^{1+d},\ c(t)>0. \end{aligned} \tag{1.2}$$

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We refer to this case as the *model Klein–Gordon equation* and give a construction of the associated parametrix for the Cauchy problem, in such way that the propagation of positive-frequency and negative-frequency singularities is under control. This allows us to reformulate the microlocal spectrum condition in terms of Cauchy data. We show how to construct many non-necessarily pure Hadamard states and then characterize pure ones. We also describe classes of symplectic transformations which preserve the microlocal spectrum condition.

(2) The above results are easily extended to operators of the form $f(\partial_t^2+a(t))g$, where f and g are smooth densities. This way, we show that the problem of constructing Hadamard states is reduced to the model case above if $M=\mathbb{R}\times\mathbb{R}^d$, the metric is given by

$$g=-c(x)dt^2+h_{jk}(x)d\mathrm{x}^j d\mathrm{x}^k, \tag{1.3}$$

and the Klein-Gordon operator is of the form

$$\begin{aligned}P(x,D_x)= \quad & c^{-\frac{1}{2}}|h|^{-\frac{1}{2}}(\partial_t+\mathrm{i}V)c^{-\frac{1}{2}}|h|^{\frac{1}{2}}(\partial_t+\mathrm{i}V)\\ & -c^{-\frac{1}{2}}|h|^{-\frac{1}{2}}(\partial_j+\mathrm{i}A_j)c^{\frac{1}{2}}|h|^{\frac{1}{2}}h^{jk}(\partial_k+\mathrm{i}A_k)+\rho,\end{aligned}$$

where $A_\mu(x)=(V(x),\mathrm{A}_j(x))$, $|h|=\det[h_{jk}]$, $[h^{jk}]=[h_{jk}]^{-1}$ and the following hypotheses are assumed:

$$\begin{aligned}&\forall\, I\subset\mathbb{R} \text{ compact interval } \exists\, C>0 \text{ such that}\\ &C\leq c(x),\ C\mathbb{1}\leq[h_{jk}(x)], \text{uniformly for } x\in I\times\mathbb{R}^d,\\ &h_{jk}(x),\ c(x),\ \rho(x), A_\mu(x)\in C^\infty(\mathbb{R},C^\infty_{\rm bd}(\mathbb{R}^d)).\end{aligned} \tag{1.4}$$

(3) For arbitrary space-times (and external potentials), using a suitable partition of unity, we explain how to glue together two-point functions of Hadamard states on smaller regions of the space-time into a globally-defined one. Using the results obtained for the special case above, this yields a construction of Hadamard states on arbitrary globally-hyperbolic space-times.

Let us mention that beside the construction for space-times with compact Cauchy surface due to Junker, a general existence result for Hadamard states is known [FNW], as well as a collection of various examples on specific classes of space-times. However, the existence argument of Fulling, Narcowich and Wald has the disadvantage of being highly non-explicit and requires non-local information on the space-time as an input. Those drawbacks are to a large extent avoided in our approach, as explained in Section 8. As for the known examples of Hadamard states for the Klein-Gordon equation, these include:

(i) passive states for stationary space-times (this includes ground- and KMS states) [SV1],
(ii) states constructed in [DMP3] for a subclass of asymptotically flat vacuum space-times at null infinity (see [Mo] for the proof),
(iii) states constructed in [DMP2] for a class of cosmological space-times (this includes the Bunch-Davies state on de-Sitter space-time),
(iv) so-called states of low energy for FLRW space-times [O],
(v) the so-called Unruh state [DMP1],
(vi) ground states and over-critical states for static potentials on Minkowski space-time considered in [W].

A short inquiry shows that the sets of assumptions (1.2) and (1.4) studied by us in greater detail are only partially covered by the examples above.

1.3. **Plan of the paper.** The paper is organized as follows.

In Section 2 we recall basic facts on bosonic quasi-free states. A special emphasis is put on explaining the relation between the neutral and the (less often discussed) *charged* case. In our problem, the use of microlocal analysis makes much more natural to work with complex quantities. In order to cover both cases it is sufficient to consider gauge-invariant charged quasi-free states.

Section 3 contains basic definitions and facts on the Klein-Gordon equation, wave front sets and Hadamard states.

In Section 4 we recall mostly well-known results on pseudo-differential calculus needed later on. This includes theorems on the pseudo-differential property of functions of pseudo-differential operators and several results related to Egorov's theorem. In Section 5 we specify our assumptions for the space-times (1.3) and explain the reduction to the model Klein-Gordon equation (1.1).

Section 6 sums up the construction of the parametrix for the model Klein-Gordon equation and contains a discussion of the necessarily arising ambiguities. We rely on Hilbert space methods rather than on Fourier integral operators. We introduce in Subsect. 6.4 the spaces of *positive/negative wavefront set solutions* and study their symplectic properties.

Section 7 contains the key results of the paper. Theorem 7.1 characterizes Hadamard states for the model Klein–Gordon equation in terms of their symplectically smeared two-point function λ. This allows us to construct a large class of Hadamard states in Subsect. 7.5. In Subsect. 7.3 we describe classes of symplectic transformations which preserve the microlocal spectrum condition. Stronger results are derived for pure quasi-free states in Subsect. 7.4. We introduce a 'canonical' Hadamard state, which is distinguished modulo the choice of a pseudo-differential operator r appearing in the construction of approximate solutions. In Subsect. 7.5 we briefly discuss the static case and show how the ground state and KMS states fit in our construction.

In Section 8 our construction of Hadamard states on an arbitrary globally hyperbolic space-time is presented. We include some remarks on the case of a compact Cauchy surface and compare our results with the construction from [J1] in Subsect. 8.1. Various proofs are collected in Appendix A.

2. Bosonic quasi-free states

2.1. **Notation.** If $\mathcal{X}$ is a real vector space we denote by $\mathcal{X}^{\#}$ its dual. Bilinear forms on $\mathcal{X}$ are identified with elements of $L(\mathcal{X}, \mathcal{X}^{\#})$, which leads to the notation $x_1 b x_2$ for $b \in L(\mathcal{X}, \mathcal{X}^{\#})$, $x_1, x_2 \in \mathcal{X}$. The space of symmetric (resp. anti-symmetric) bilinear forms on $\mathcal{X}$ is denoted by $L_{\rm s}(\mathcal{X}, \mathcal{X}^{\#})$ (resp. $L_{\rm a}(\mathcal{X}, \mathcal{X}^{\#})$).

If $\sigma \in L_{\rm s}(\mathcal{X}, \mathcal{X}^{*})$, we denote by $O(\mathcal{X}, \sigma)$ the linear (pseudo-)orthogonal group on $\mathcal{X}$. Similarly if $\sigma \in L_{\rm a}(\mathcal{X}, \mathcal{X}^{\#})$ is non-degenerate, i.e. $(\mathcal{X}, \sigma)$ is a symplectic space, we denote by $Sp(\mathcal{X}, \sigma)$ the linear symplectic group on $\mathcal{X}$.

If $\mathcal{X}$ is a complex vector space, we denote by $\mathcal{X}^{*}$ its anti-dual, i.e. the space of anti-linear forms on $\mathcal{X}$. Sesquilinear forms on $\mathcal{X}$ are identified with elements of $L(\mathcal{X}, \mathcal{X}^{*})$, and we use the notation $(x_1|bx_2)$ or sometimes $\overline{x_1}bx_2$ for $b \in L(\mathcal{X}, \mathcal{X}^{*})$, $x_1, x_2 \in \mathcal{X}$.

The space of hermitian (resp. anti-hermitian) bilinear forms on $\mathcal{X}$ is denoted by $L_{\rm s}(\mathcal{X}, \mathcal{X}^{*})$ (resp. $L_{\rm a}(\mathcal{X}, \mathcal{X}^{*})$).

If $q \in L_{\rm s}(\mathcal{X}, \mathcal{X}^{*})$ is non-degenerate, i.e. $(\mathcal{X}, q)$ is a pseudo-unitary space, we denote by $U(\mathcal{X}, q)$ the linear pseudo-unitary group on $\mathcal{X}$.

If b is a bilinear form on the real vector space $\mathcal{X}$, its canonical sesquilinear extension to $\mathbb{C}\mathcal{X}$ is by definition the sesquilinear form $b_{\mathbb{C}}$ on $\mathbb{C}\mathcal{X}$ given by

$$(w_1|b_{\mathbb{C}}w_2) := x_1 b x_2 + y_1 b y_2 + {\rm i} x_1 b y_2 - {\rm i} y_1 b x_2, \quad w_i = x_i + {\rm i} y_i$$

for $x_i, y_i \in \mathcal{X}$, $i = 1, 2$. This extension maps (anti-)symmetric forms on $\mathcal{X}$ onto (anti-)hermitian forms on $\mathbb{C}\mathcal{X}$.

Conversely if $\mathcal{X}$ is a complex vector space and $\mathcal{X}_{\mathbb{R}}$ is its real form, i.e. $\mathcal{X}$ considered as a real vector space, then for $b \in L_{\rm s/a}(\mathcal{X}, \mathcal{X}^*)$ the form ${\rm Re}b$ belongs to $L_{\rm s/a}(\mathcal{X}_{\mathbb{R}}, \mathcal{X}_{\mathbb{R}}^{\#})$.

2.2. **Bosonic quasi-free states, neutral case.** Let $(\mathcal{X}, \sigma)$ be a real symplectic space, i.e. a pair consisting of a real vector space $\mathcal{X}$ and a non-degenerate anti-symmetric form $\sigma \in L_{\rm a}(\mathcal{X}, \mathcal{X}^{\#})$.

We denote $\mathcal{A}(\mathcal{X}, \sigma)$ the Weyl CCR C^*-algebra of $(\mathcal{X}, \sigma)$, formally generated by elements of the form $W(y)$ for $y \in \mathcal{X}$, with:

$$W(y)^* = W(-y), \quad W(x)W(y) = {\rm e}^{-{\rm i}(x\sigma y)/2} W(x+y), \quad x, y \in \mathcal{X}.$$

Definition 2.1. *A state ω on $\mathcal{A}(\mathcal{X}, \sigma)$ is called a (bosonic, neutral) quasi-free state if there is a symmetric form η (called the* covariance *of ω) on $\mathcal{X}$ such that*

$$\omega(W(x)) = {\rm e}^{-\frac{1}{2}x\eta x}, \qquad x \in \mathcal{X}.$$

A quasi-free state ω on $\mathcal{A}(\mathcal{X}, \sigma)$ is regular, i.e. the field operators $\phi(x)$ are well-defined as selfadjoint operators in the GNS representation of ω with:

$$[\phi(x_1), \phi(x_2)] = {\rm i}(x_1\sigma x_2)\mathbb{1}, \text{ as quadratic forms on } {\rm Dom}\phi(x_1) \cap {\rm Dom}\phi(x_2),$$

and:

$$\omega(\phi(x_1)\phi(x_2)) = x_1\eta x_2 + \frac{\rm i}{2}x_1\sigma x_2, \quad x_1, x_2 \in \mathcal{X}. \tag{2.1}$$

It is convenient to introduce the sesquilinear hermitian form

$$q := {\rm i}\sigma_{\mathbb{C}},$$

usually called the *charge* and

$$\lambda := \eta_{\mathbb{C}} + \frac{1}{2}q \in L_{\rm s}(\mathbb{C}\mathcal{X}, \mathbb{C}\mathcal{X}^*).$$

The following results are well-known (see e.g. [DG, Chaps. 17,11]).

Proposition 2.2. *Let $\eta \in L_{\rm s}(\mathcal{X}, \mathcal{X}^{\#})$. Then the following are equivalent:*
(1) *η is the covariance of a quasi-free state on $\mathcal{A}(\mathcal{X}, \sigma)$,*
(2) *$x\eta x \geq 0$, $|x_1\sigma x_2| \leq 2(x_1\eta x_1)^{\frac{1}{2}}(x_2\eta x_2)^{\frac{1}{2}}$, $x_1, x_2 \in \mathcal{X}$,*
(3) *$\lambda \geq 0$ on $\mathbb{C}\mathcal{X}$,*
(4) *$\lambda \geq 0$, $\lambda \geq q$ on $\mathbb{C}\mathcal{X}$.*

Proposition 2.3. *Let $\eta \in L_{\rm s}(\mathcal{X}, \mathcal{X}^{\#})$. Then the following are equivalent:*
(1) *η is the covariance of a* pure *quasi-free state on $\mathcal{A}(\mathcal{X}, \sigma)$,*
(2) *$(2\eta, \sigma)$ is* Kähler*, i.e. there exists an anti-involution ${\rm j}_1 \in Sp(\mathcal{X}, \sigma)$ such that $2\eta = \sigma {\rm j}_1$.*

Proposition 2.4. *Let η_1, η_2 be covariances of two pure quasi-free states on $\mathcal{A}(\mathcal{X}, \sigma)$. Then there exists $r \in Sp(\mathcal{X}, \sigma)$ such that $\eta_2 = r^{\#}\eta_1 r$.*

2.3. **Gauge-invariant bosonic quasi-free states.** Let us now consider the case of a complex symplectic space $(\mathcal{Y}, \sigma)$, i.e. a pair consisting of a complex vector space $\mathcal{Y}$ and a non-degenerate anti-hermitian form $\sigma \in L_{\rm a}(\mathcal{Y}, \mathcal{Y}^*)$. The complex structure on $\mathcal{Y}$ will be denoted by j, to distinguish it from the complex number ${\rm i} \in \mathbb{C}$.

As before we introduce the charge $q := {\rm i}\sigma$ which is hermitian.

Note that $(\mathcal{Y}_{\mathbb{R}}, {\rm Re}\sigma)$ is a real symplectic space with ${\rm j} \in Sp(\mathcal{Y}_{\mathbb{R}}, {\rm Re}\sigma)$. Conversely if $(\mathcal{X}, \sigma)$ is a real symplectic space equipped with an anti-involution ${\rm j} \in Sp(\mathcal{X}, \sigma)$,

then denoting by $\mathcal{Y}$ the space $\mathcal{X}$ equipped with the complex structure j and setting $(x_1|\hat{\sigma}x_2) := x_1\sigma x_2 - \mathrm{i}x_1\sigma \mathrm{j}x_2$, the space $(\mathcal{Y}, \hat{\sigma})$ is a complex symplectic space.

For coherence of notation we will denote the Weyl CCR algebra $\mathcal{A}(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$ by $\mathcal{A}(\mathcal{Y}, \sigma)$.

Let us now consider a quasi-free state ω on $\mathcal{A}(\mathcal{Y}, q)$, as in Subsect. 2.2. The state ω is called *gauge-invariant* if

$$\omega(W(y)) = \omega(W(\mathrm{e}^{\mathrm{j}\theta}y)), \quad 0 \leq \theta < 2\pi, \quad y \in \mathcal{Y}.$$

If η is the covariance of ω then ω is gauge-invariant iff $\mathrm{j} \in U(\mathcal{Y}_{\mathbb{R}}, \eta)$. If the state ω is not gauge-invariant, the complex structure j plays no role and one can forget it. One is then reduced to the situation of Subsect. 2.2.

Let now $\phi(y)$ for $y \in \mathcal{Y}$ be the selfadjoint fields in the GNS representation of ω. One can introduce the *charged fields*:

$$\psi(y) := \frac{1}{\sqrt{2}}(\phi(y) + \mathrm{i}\phi(\mathrm{j}y)),\ \psi^*(y) := \frac{1}{\sqrt{2}}(\phi(y) - \mathrm{i}\phi(\mathrm{j}y)),\ y \in \mathcal{Y}.$$

The map $\mathcal{Y} \ni y \mapsto \psi^*(y)$ (resp. $\mathcal{Y} \ni y \mapsto \psi(y)$) is $\mathbb{C}-$linear (resp. $\mathbb{C}-$anti-linear). The commutation relations take the form:

$$[\psi(y_1), \psi(y_2)] = [\psi^*(y_1), \psi^*(y_2)] = 0,\ [\psi(y_1), \psi^*(y_2)] = (y_1|qy_2)\mathbb{1},\ y_1, y_2 \in \mathcal{Y}.$$

If ω is a gauge-invariant quasi-free state on $\mathcal{A}(\mathcal{Y}, q)$, then:

$$\begin{aligned} \omega(\psi(y_1)\psi(y_2)) = &\quad \omega(\psi^*(y_1)\psi^*(y_2)) = 0, \\ \omega(\psi(y_1)\psi^*(y_2)) =: &\quad (y_1|\lambda y_2),\ y_1, y_2 \in \mathcal{Y}. \end{aligned} \tag{2.2}$$

We will call $\lambda \in L_{\mathrm{s}}(\mathcal{Y}, \mathcal{Y}^*)$ the *(complex) two-point function* of the gauge invariant quasi-free state ω.

Sometimes one considers instead of λ the *density* or *complex covariance* c defined by

$$(y_1|cy_2) := \omega(\psi^*(y_2)\psi(y_1)).$$

Clearly $\lambda = c + q$.

The following propositions are the analogues of Props. 2.2, 2.3, 2.4. We sketch their proofs for the reader's convenience.

Proposition 2.5. *Let $\lambda \in L_{\mathrm{s}}(\mathcal{Y}, \mathcal{Y}^*)$. Then the following are equivalent:*

(1) *λ is the two-point function of a gauge-invariant quasi-free state on $\mathcal{A}(\mathcal{Y}, q)$,*
(2) *$\lambda \geq 0$, $\lambda \geq q$.*

Proof. Introducing the selfadjoint fields $\phi(y)$ we obtain that

$$\omega(\phi(y_1)\phi(y_2)) = \mathrm{Re}(y_1|(\lambda - \frac{1}{2}q)y_2) + \frac{\mathrm{i}}{2}\mathrm{Re}(y_1|\sigma y_2).$$

Therefore we have $\eta = \mathrm{Re}(\lambda - \frac{1}{2}q)$. Since ω is gauge-invariant we have

$$\mathrm{j} \in O(\mathcal{Y}_{\mathbb{R}}, \eta) \cap Sp(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma) = O(\mathcal{Y}_{\mathbb{R}}, \eta) \cap O(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}q).$$

From this fact we deduce that $\eta \geq 0 \Leftrightarrow \lambda \geq \frac{1}{2}q$, and that the second condition in Prop. 2.2 (with σ replaced by $\mathrm{Re}\sigma$) is equivalent to

$$\pm q \leq 2\lambda - q.$$

These three conditions are equivalent to $\lambda \geq 0$, $\lambda \geq q$. $\Box$

Proposition 2.6. *Let $\lambda \in L_{\mathrm{s}}(\mathcal{Y}, \mathcal{Y}^*)$. Then the following are equivalent:*

(1) *λ is the two-point function of a* pure *gauge-invariant quasi-free state on $\mathcal{A}(\mathcal{Y}, q)$,*
(2) *there exists an involution $\kappa \in U(\mathcal{Y}, q)$ such that $q\kappa \geq 0$ and $\lambda = \frac{1}{2}q(\mathbb{1} + \kappa)$.*
(3) *$\lambda \geq \frac{1}{2}q$, $\lambda q^{-1}\lambda = \lambda$.*

Proof. By Prop. 2.3 the state ω is pure iff there exists an anti-involution $\mathrm{j}_1 \in Sp(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$ such that

$$2\eta = (\mathrm{Re}\sigma)\mathrm{j}_1. \tag{2.3}$$

Since $\mathrm{j} \in O(\mathcal{Y}_{\mathbb{R}}, \eta) \cap Sp(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$ we obtain that $\mathrm{j}_1 \in U(\mathcal{Y}, q)$, i.e. j_1 is $\mathbb{C}-$linear and pseudo-unitary for q. From (2.3) we then get that $2\lambda - q = \sigma\mathrm{j}_1$. Setting $\kappa = -\mathrm{j}\mathrm{j}_1$ we see that $\kappa \in U(\mathcal{Y}, q)$ and $\lambda = \frac{1}{2}q(\mathbb{1} + \kappa)$. Therefore (1) is equivalent to

$$(4)\ \lambda \geq 0,\ \lambda \geq q,\ \lambda = \frac{1}{2}q(\mathbb{1} + \kappa),\ \kappa^2 = \mathbb{1}, \kappa \in U(\mathcal{Y}, q).$$

(4) clearly implies (2). Let us prove the converse implication. Set $P_{\pm} := \frac{1}{2}(\mathbb{1} \pm \kappa)$. Clearly $P_{\pm}$ are projections with $P_{\pm}^* q = qP_{\pm}$, $\kappa P_{\pm} = \pm P_{\pm}$, and

$$\lambda \geq 0,\ \lambda \geq q \Leftrightarrow \pm qP_{\pm} \geq 0.$$

Now we have

$$qP_{\pm} = qP_{\pm}^2 = P_{\pm}^* qP_{\pm} = \pm P_{\pm}^* q\kappa P_{\pm},$$

which completes the proof since $q\kappa \geq 0$. The fact that (2) and (3) are equivalent is an easy computation. □

Proposition 2.7. *Let λ_1, λ_2 be two-point functions of two pure, gauge-invariant quasi-free states on $\mathcal{A}(\mathcal{Y}, q)$. Then there exists $r \in U(\mathcal{Y}, q)$ such that $\lambda_2 = r^*\lambda_1 r$.*

Proof. We introduce the real covariances η_1, η_2. By Prop. 2.4 there exists $r \in Sp(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$ with $\eta_2 = r^{\#}\eta_1 r$. Using the gauge-invariance of the two states we obtain that $r\mathrm{j} = \mathrm{j}r$, hence $r \in U(\mathcal{Y}, q)$. □

2.4. **Complexification of bosonic quasi-free states.** Let now $(\mathcal{X}, \sigma)$ be a real symplectic space. We set $\mathcal{Y} := \mathbb{C}\mathcal{X}$, denoting by j the canonical complex structure on $\mathbb{C}\mathcal{X}$, and equip $\mathcal{Y}$ with $\sigma_{\mathbb{C}}$, obtaining a complex symplectic space. We set as in Subsect. 2.3 $q = \mathrm{i}\sigma_{\mathbb{C}}$.

Clearly $(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma_{\mathbb{C}})$ is isomorphic to $(\mathcal{X} \oplus \mathcal{X}, \sigma \oplus \sigma)$ as real symplectic spaces. If ω is a quasi-free state on $(\mathcal{X}, \sigma)$ with covariance η, then we can consider the quasi-free state $\tilde{\omega}$ on $(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma_{\mathbb{C}})$ with covariance $\mathrm{Re}\eta_{\mathbb{C}}$.

It is easy to see that $\tilde{\omega}$ is gauge-invariant, and its (complex) two-point function λ is equal to

$$\lambda = \eta_{\mathbb{C}} + \frac{1}{2}q.$$

Therefore by complexifying a quasi-free state ω on a real symplectic space $(\mathcal{X}, \sigma)$, we obtain a gauge-invariant quasi-free state $\tilde{\omega}$ on $(\mathrm{Re}\mathbb{C}\mathcal{X}, \mathrm{Re}\sigma_{\mathbb{C}})$. It follows that, possibly after complexifying the real symplectic space $(\mathcal{X}, \sigma)$, one can always restrict the discussion to gauge-invariant quasi-free states.

In the sequel we will henceforth only consider gauge-invariant quasi-free states, and often call them simply quasi-free states.

3. Hadamard states

3.1. **Klein-Gordon equations on a globally hyperbolic space time.** Consider a globally hyperbolic space-time $(M, g_{\mu\nu}dx^{\mu}dx^{\nu})$. We use the convention $(-, +, \cdots, +)$ for the signature.

We use the notations

$$|g| := \det[g_{\mu\nu}], \quad [g^{\mu\nu}] := [g_{\mu\nu}]^{-1}, \quad dv := |g|^{\frac{1}{2}}dx.$$

If S is a Cauchy hypersurface, we denote by n^{ν} the unit future directed normal vector field to S (after choosing a time orientation), and by ds the surface measure on S obtained from dv.

We fix a smooth vector potential $A_\mu(x)dx^\mu$ and a smooth function $\rho : M \to \mathbb{R}$. The associated Klein-Gordon operator is:

$$P(x, D_x) = |g|^{-\frac{1}{2}}(\partial_\mu + \mathrm{i}A_\mu)|g|^{\frac{1}{2}}g^{\mu\nu}(\partial_\nu + \mathrm{i}A_\nu) + \rho. \tag{3.4}$$

We equip $\mathcal{D}(M)$ with the scalar product

$$(u_1|u_2) = \int_M \overline{u}_1 u_2 dv,$$

so that $P(x, D_x)$ is formally selfadjoint. We denote by $E_\pm$ the *retarded/advanced fundamental solutions* of $P(x, D_x)$, and by $E = E_+ - E_-$ the *Pauli-Jordan commutator function* Recall that $E_\pm^* = E_\mp$ hence $E = -E^*$.

A function u on M is called *space-compact* if the intersection of $\mathrm{supp}\, u$ with any Cauchy hypersurface of M is compact. The space of smooth space-compact functions will be denoted by $C^\infty_{\mathrm{sc}}(M)$.

We denote by $\mathrm{Sol}_{C^\infty}(P) \subset C^\infty(M)$ the space of smooth space-compact solutions of

$$\text{(KG)} \quad P(x, D_x)\phi = 0.$$

One has (see e.g. [BGP]):

$$\mathrm{Sol}_{C^\infty}(P) = E\mathcal{D}(M). \tag{3.5}$$

Moreover if we fix a Cauchy hypersurface S and set

$$\begin{array}{rll} \rho : & \mathrm{Sol}_{C^\infty}(P) & \to \mathcal{D}(S) \oplus \mathcal{D}(S) \\ & \phi & \mapsto (\phi_{|S}, \mathrm{i}^{-1} n^\mu (\nabla_\mu + \mathrm{i}A_\mu)\phi_{|S}) =: (\rho_0\phi, \rho_1\phi), \end{array}$$

then $\rho : \mathrm{Sol}_{C^\infty}(P) \to \mathcal{D}(S) \oplus \mathcal{D}(S)$ is bijective (see e.g. [BGP]).

Using $\rho \circ E$ we can identify sesquilinear forms on $\mathcal{D}(S) \oplus \mathcal{D}(S)$ with sesquilinear forms on $\mathcal{D}(M)/\mathrm{Ker}E$: if c is a sesquilinear form on $\mathcal{D}(S) \oplus \mathcal{D}(S)$, we set:

$$([u]|C[v]) := ((\rho \circ E)u|c(\rho \circ E)v), \; u, v \in \mathcal{D}(M). \tag{3.6}$$

Let ς be the sesquilinear form on $\mathcal{D}(M)/\mathrm{Ker}E$ defined by

$$([u]|\varsigma[v]) := \langle \overline{u}, Ev \rangle = \langle E, \overline{u} \otimes v \rangle, \quad u, v \in \mathcal{D}(M).$$

By construction $(\mathcal{D}(M)/\mathrm{Ker}E, \varsigma)$ is a complex symplectic space. Setting also

$$(f|\sigma g) := -\mathrm{i} \int_S (\overline{f_0} g_1 + \overline{f_1} g_0) ds, \; f, g \in \mathcal{D}(S) \oplus \mathcal{D}(S),$$

we have

$$([u]|\varsigma[v]) = (\rho \circ Eu|\sigma(\rho \circ Ev), \tag{3.7}$$

i.e. σ is identified with ς under (3.6).

We consider quasi-free states on $\mathcal{A}(\mathcal{D}(M, \mathbb{R})/\mathrm{Ker}E, \varsigma)$ in the neutral case and gauge-invariant quasi-free states on $\mathcal{A}(\mathcal{D}(M)/\mathrm{Ker}E, \varsigma)$ in the charged case.

If λ is the two-point function of a gauge-invariant quasi-free state on $\mathcal{A}(\mathcal{D}(S) \oplus \mathcal{D}(S), \sigma)$ then the two-point function on $\mathcal{A}(\mathcal{D}(M)/\mathrm{Ker}E, \varsigma)$ obtained from (3.6) will be denoted by Λ.

3.2. **The wave front set.** Let M be a smooth manifold. As usual $\mathcal{E}(M)$ is the space of smooth functions on M, $\mathcal{D}(M)$ the space of smooth compactly supported functions on M, $\mathcal{D}'(M)$ the space of distributions on M and $\mathcal{E}'(M)$ the space of compactly supported distributions.

We denote by T^*M be the cotangent bundle of M. The zero section of T^*M will be denoted by Z.

3.2.1. *Operations on conic sets.* A set $\Gamma \subset T^*M\backslash Z$ is *conic* if

$$(x,\xi)\in\Gamma \Rightarrow (x,t\xi)\in\Gamma,\ \forall\, t>0.$$

If $\Gamma \subset T^*M\backslash Z$ is conic, we set:

$$-\Gamma := \{(x,-\xi):\ (x,\xi)\in\Gamma\}.$$

Let M_i, $i=1,2$ be two manifolds, Z_i the zero section of T^*M_i and $\Gamma\subset T^*(M_1\times M_2)\backslash Z$ be a conic set. The elements of $T^*(M_1\times M_2)\backslash Z$ will be denoted by (x_1,ξ_1,x_2,ξ_2), which allows to consider Γ as a relation between T^*M_2 and T^*M_1, still denoted by Γ. Clearly Γ maps conic sets into conic sets. We set:

$$\Gamma' := \{(x_1,\xi_1,x_2,-\xi_2):\ (x_1,\xi_1,x_2,\xi_2)\in\Gamma\}\subset T^*(M_1\times M_2)\backslash Z,$$

$$\mathrm{Exch}(\Gamma) := \{(x_2,\xi_2,x_1,\xi_1):\ (x_1,\xi_1,x_2,\xi_2)\in\Gamma\}\subset T^*(M_2\times M_1)\backslash Z,$$

$${}_{M_1}\Gamma := \{(x_1,\xi_1):\ \exists\, x_2 \text{ such that } (x_1,\xi_1,x_2,0)\in\Gamma\} = \Gamma(Z_2)\subset T^*M_1\backslash Z_1,$$

$$\Gamma_{M_2} := \{(x_2,\xi_2):\ \exists\, x_1 \text{ such that } (x_1,0,x_2,\xi_2)\in\Gamma\} = \Gamma^{-1}(Z_1)\subset T^*M_2\backslash Z_2.$$

3.2.2. *Properties of the wave front set.* Recall that if $u\in\mathcal{D}'(M)$ then the wave front set $\mathrm{WF}(u)$ is a conic subset of $T^*M\backslash Z$. We refer to [H1] for the exact definition and the proof of the following basic properties:

(1) **Complex conjugation**: if $u\in\mathcal{D}'(M)$ then $\mathrm{WF}(\overline{u}) = -\mathrm{WF}(u)$.

(2) **Restriction to a sub-manifold**: let $S\subset M$ a sub-manifold. The *co-normal bundle* to S in M is:

$$T^*_S M := \{(x,\xi)\in T^*M\backslash Z:\ x\in S,\ \xi\cdot v = 0\ \forall v\in T_xS\}.$$

If $u\in\mathcal{D}'(M)$, the restriction $u_{|S}$ of u to S is well defined if $\mathrm{WF}(u)\cap T^*_SM=\emptyset$. One has

$$\mathrm{WF}(u_{|S})\subset\{(x,\xi_{|T_xS}):\ x\in S,\ (x,\xi)\in\mathrm{WF}(u)\}.$$

(3) **Kernels**: let $K:\mathcal{D}(M_2)\to\mathcal{D}'(M_1)$ be linear continuous and denote by $K(x_1,x_2)\in\mathcal{D}'(M_1\times M_2)$ its distributional kernel. Then Ku is well defined for $u\in\mathcal{E}'(M_2)$ if $\mathrm{WF}(u)\cap\mathrm{WF}(K)'_{M_2}=\emptyset$ and in such case

$$\mathrm{WF}(Ku)\subset\ {}_{M_1}\mathrm{WF}(K)\cup\mathrm{WF}(K)'\circ\mathrm{WF}(u).$$

(4) **Composition**: let $K_1\in\mathcal{D}'(M_1\times M_2)$, $K_2\in\mathcal{D}'(M_2\times M_3)$, where K_2 is properly supported, i.e. the projection: $\mathrm{supp}\,K_2\to M_2$ is proper. Then $K_1\circ K_2$ is well defined if

$$\mathrm{WF}(K_1)'_{M_2}\ \cap\ {}_{M_2}\mathrm{WF}(K_2)'=\emptyset,$$

and in such case

$$\mathrm{WF}(K_1\circ K_2)'\subset\mathrm{WF}(K_1)'\circ\mathrm{WF}(K_2)'\ \cup\ {}_{M_1}\mathrm{WF}(K_1)'\times Z_3\ \cup\ Z_1\times\mathrm{WF}(K_2)'_{M_3}.$$

(5) **Adjoint:** let us denote by K^* the adjoint of K with respect to any smooth non-vanishing density dx on M. Then

$$\mathrm{WF}(K^*)' = \mathrm{Exch}(\mathrm{WF}(K)').$$

3.3. **Distinguished parametrices and microlocal spectrum condition.** Let us recall basic elements of the theory of distinguished parametrices of Duistermaat and Hörmander [DH] for the case of the Klein-Gordon operator $P(x,D)$. The *characteristic manifold* of $P(x,D)$ is

$$\mathcal{N} := \{(x,\xi)\in T^*M\backslash Z:\ p(x,\xi)=0\},$$

where $p(x,\xi)=g^{\mu\nu}(x)\xi_\mu\xi_\nu$ is the principal symbol of $P(x,D)$.

We use the notation $X = (x, \xi)$ for points in $T^*M\backslash Z$. We write $X_1 \sim X_2$ if $X_1 = (x_1, \xi_1)$ and $X_2 = (x_2, \xi_2)$ are in $\mathcal{N}$ and X_1 and X_2 are on the same Hamiltonian curve for p.

Let us denote by $V_{x\pm} \subset T_xM$ for $x \in M$, the open future/past light cones and $V^*_{x\pm}$ the dual cones

$$V^*_{x\pm} := \{\xi \in T^*_xM : \ \xi \cdot v > 0, \ \forall v \in V_{x\pm}, \ v \neq 0\}.$$

The set $\mathcal{N}$ has two connected components invariant under the Hamiltonian flow of p, namely:

$$\mathcal{N}_\pm := \{X \in \mathcal{N} : \ \xi \in V^*_{x\pm}\}.$$

Recall that $E_\pm$ denote respectively the retarded and advanced fundamental solution. We denote respectively $E_{\rm F}$, $E_{\overline{\rm F}}$ the Feynman and anti-Feynman parametrix. The theory of Duistermaat and Hörmander provides among others a description of the wave front sets of the parametrices $E_\pm$, $E_{\rm F}$, $E_{\overline{\rm F}}$ and establishes their uniqueness up to smooth functions. The proof of the next lemma can be found for instance in [J1, Thm. 2.29].

Lemma 3.1. *We have:*

$$\begin{array}{ll}(1) & {\rm WF}(E)' = \{(X_1, X_2) \in \mathcal{N} \times \mathcal{N} : \quad X_1 \sim X_2\},\\ (2) & {\rm WF}(E_+ - E_{\rm F})' = \{(X_1, X_2) \in \mathcal{N}_- \times \mathcal{N}_- : \quad X_1 \sim X_2\},\\ (3) & {\rm WF}(E_- - E_{\rm F})' = \{(X_1, X_2) \in \mathcal{N}_+ \times \mathcal{N}_+ : \quad X_1 \sim X_2\}.\end{array}$$

We are now ready to formulate the microlocal spectrum condition.

Definition 3.2. *Let $\Lambda : \mathcal{D}(M) \to \mathcal{D}'(M)$ be linear continuous. Then Λ satisfies the* microlocal spectrum condition *if*

$$(\mu{\rm sc}) \qquad {\rm WF}(\Lambda)' \subset \{(X_1, X_2) \in \mathcal{N}_+ \times \mathcal{N}_+ : \quad X_1 \sim X_2\}.$$

A (neutral or charged, gauge invariant) quasi-free state is a Hadamard state *if its two-point function Λ satisfies the microlocal spectrum condition.*

Remark 3.3. *If instead of Λ we consider the charge density $C = \Lambda - Q$, then it is easy to deduce using Radzikowski's theorem* [R] *and Lemma 3.1 that the corresponding condition for C is*

$${\rm WF}(C)' \subset \{(X_1, X_2) \in \mathcal{N}_- \times \mathcal{N}_- : \quad X_1 \sim X_2\}.$$

One can also show that the inclusion in (μsc) and the one above can be replaced by equalities.

4. Background on pseudo-differential calculus

4.1. **Notation.** - If $f : \mathbb{R}_t \times \mathbb{R}^n_x \to \mathbb{C}$ is a function, and $t \in \mathbb{R}$ we denote by $f(t)$ the function:

$$f(t) : \ \mathbb{R}^n \ni x \mapsto f(t, x) \in \mathbb{C}.$$

- We denote by $C^\infty_{\rm bd}(\mathbb{R}^n)$ the space of smooth functions on $\mathbb{R}^n$ uniformly bounded with all derivatives. We equip $C^\infty_{\rm bd}(\mathbb{R}^n)$ with its canonical Fréchet space structure. We denote by $H^m(\mathbb{R}^d)$ the Sobolev space of order $m \in \mathbb{R}$.

- We denote by $\mathcal{S}(\mathbb{R}^d)$, resp. $\mathcal{S}'(\mathbb{R}^d)$ the space of Schwartz functions, resp. distributions on $\mathbb{R}^d$.

- We set

$$\mathcal{H}(\mathbb{R}^d) := \cap_{m\in\mathbb{R}} H^m(\mathbb{R}^d), \ \mathcal{H}'(\mathbb{R}^d) := \cup_{m\in\mathbb{R}} H^m(\mathbb{R}^d),$$

equipped with their canonical topologies.

- If E, F are two topological vector spaces, we write $A : E \to F$ if A is linear continuous from E to F.

- We set $D_x = {\rm i}^{-1}\partial_x$, $\langle x\rangle = (1 + x^2)^{\frac12}$, $x \in \mathbb{R}^d$.

4.2. **Symbol classes.** We denote by $S^m(\mathbb{R}^{2d})$, $m\in\mathbb{R}$ the symbol class

$$a\in S^m(\mathbb{R}^{2d}) \ \text{ if } \ \partial_x^\alpha\partial_k^\beta a(x,k)\in O(\langle k\rangle^{m-|\beta|}),\ \alpha,\beta\in\mathbb{N}^d. \tag{4.8}$$

Similarly we will denote by $S^m(\mathbb{R})$ the class

$$f\in S^m(\mathbb{R}) \text{ if } \partial_\lambda^\alpha f(\lambda)\in O(\langle\lambda\rangle^{m-\alpha}),\ \alpha\in\mathbb{N}. \tag{4.9}$$

We denote by $S^m_{\rm h}(\mathbb{R}^{2d})$ the subspace of $S^m(\mathbb{R}^{2d})$ of symbols homogeneous of degree m in the k variable:

$$a\in S^m_{\rm h}(\mathbb{R}^{2d}) \text{ if } a\in S^m(\mathbb{R}^{2d}) \text{ and } a(x,\lambda k)=\lambda^m a(x,k),\ \lambda\geq 1,\ |k|\geq 1. \tag{4.10}$$

We set

$$S^{-\infty}(\mathbb{R}^{2d}):=\bigcap_{m\in\mathbb{R}}S^m(\mathbb{R}^{2d}).$$

If $a_{m-k}\in S^{m-k}(\mathbb{R}^{2d})$ for $k\in\mathbb{N}$ and $a\in S^m(\mathbb{R}^{2d})$ we write

$$a\sim\sum_{k=0}^\infty a_{m-k}$$

if

$$a-\sum_{k=0}^n a_{m-k}\in S^{m-n-1}(\mathbb{R}^{2d}),\ \forall n\in\mathbb{N}. \tag{4.11}$$

Note that if $a_{m-k}\in S^{m-k}(\mathbb{R}^{2d})$ for $k\in\mathbb{N}$, then it is well-known that there exists $a\in S^m(\mathbb{R}^{2d})$, unique modulo $S^{-\infty}(\mathbb{R}^{2d})$, such that $a\sim\sum_{k=0}^\infty a_{m-k}$.

We say that a symbol $a\in S^m(\mathbb{R}^{2d})$ is *poly-homogeneous* if $a\sim\sum_{k=0}^\infty a_{m-k}$ for $a_{m-k}\in S^{m-k}_{\rm h}(\mathbb{R}^{2d})$.The symbols a_{m-k} are then clearly unique. The subspace of *poly-homogeneous symbols* of degree m will be denoted by $S^m_{\rm ph}(\mathbb{R}^{2d})$. The space $S^m_{\rm ph}(\mathbb{R})\subset S^m(\mathbb{R})$ is defined similarly.

We will often write $S^m_{\rm (ph)}$ for $S^m_{\rm (ph)}(\mathbb{R}^{2d})$. We equip $S^m_{\rm (ph)}(\mathbb{R}^{2d})$ with the Fréchet space topology given by the semi-norms:

$$\|a\|_{m,N}:=\sup_{|\alpha|+|\beta|\leq N}|\langle k\rangle^{-m+|\beta|}\partial_x^\alpha\partial_k^\beta a|.$$

We set

$$S^\infty_{\rm (ph)}(\mathbb{R}^{2d}):=\bigcup_{m\in\mathbb{R}}S^m_{\rm (ph)}(\mathbb{R}^{2d}).$$

4.3. **Principal symbol and characteristic set.** The *principal symbol* of $a\in S^m$, denoted by $\sigma_{\rm pr}(a)$ is the equivalence class $a+S^{m-1}$ in S^m/S^{m-1}. If $a\in S^m_{\rm ph}$ then $a+S^{m-1}$ has a unique representative in $S^m_{\rm h}$, namely the function a_m in (4.11). Therefore in this case the principal symbol is a function on $\mathbb{R}^{2d}$, homogeneous of degree m in k.

The *characteristic set* of $a\in S^m_{\rm ph}$ is defined as

$$\mathrm{Char}(a):=\{(x,k)\in T^*\mathbb{R}^d\backslash\{0\}:\ a_m(x,k)=0\}, \tag{4.12}$$

it is clearly conic in the k variable.

A symbol $a\in S^m(\mathbb{R}^{2d})$ is *elliptic* if there exists $C,R>0$ such that

$$|a(x,k)|\geq C\langle k\rangle^m,\ |k|\geq R.$$

Clearly $a\in S^m_{\rm ph}(\mathbb{R}^{2d})$ is elliptic iff $\mathrm{Char}(a)=\emptyset$.

4.4. **Pseudo-differential operators.** In this subsection we collect some well-known results about pseudo-differential calculus.

For $a \in S^m(\mathbb{R}^{2d})$, we denote by $\mathrm{Op}^{\mathrm{w}}(a)$ the *Weyl quantization* of a defined by:

$$\mathrm{Op}^{\mathrm{w}}(a)u(x) = a^{\mathrm{w}}(x, D)u(x) := (2\pi)^{-d} \iint \mathrm{e}^{\mathrm{i}(x-y)k} a(\frac{x+y}{2}, k)u(y)\mathrm{d}y\mathrm{d}k.$$

One has $\mathrm{Op}^{\mathrm{w}}(a) : \mathcal{H}(\mathbb{R}^d) \to \mathcal{H}(\mathbb{R}^d)$ and

$$\mathrm{Op}^{\mathrm{w}}(a)^* = \mathrm{Op}^{\mathrm{w}}(\overline{a}),$$

hence $\mathrm{Op}^{\mathrm{w}}(a) : \mathcal{H}'(\mathbb{R}^d) \to \mathcal{H}'(\mathbb{R}^d)$.

We denote by $\Psi^m_{(\mathrm{ph})}(\mathbb{R}^d)$ the space $\mathrm{Op}^{\mathrm{w}}(S^m_{(\mathrm{ph})}(\mathbb{R}^{2d}))$ and set

$$\Psi^\infty_{(\mathrm{ph})}(\mathbb{R}^d) = \bigcup_{m\in\mathbb{R}} \Psi^m_{(\mathrm{ph})}(\mathbb{R}^d),\ \Psi^{-\infty}(\mathbb{R}^d) = \bigcap_{m\in\mathbb{R}} \Psi^m(\mathbb{R}^d).$$

We will often write $\Psi^m_{(\mathrm{ph})}$ instead of $\Psi^m_{(\mathrm{ph})}(\mathbb{R}^d)$. We will equip $\Psi^m_{(\mathrm{ph})}(\mathbb{R}^d)$ with the Fréchet space topology obtained from the topology of $S^m(\mathbb{R}^{2d})$.

If $a = a^{\mathrm{w}}(x, D_x) \in \Psi^m_{\mathrm{ph}}(\mathbb{R}^d)$ the $m-$homogeneous function $\sigma_{\mathrm{pr}}(a) =: a_m(x, k)$ is called the *principal symbol* of a.

Let $s, m \in \mathbb{R}$. Then the map

$$S^m(\mathbb{R}^d) \ni a \mapsto \mathrm{Op}^{\mathrm{w}}(a) \in B(H^s(\mathbb{R}^d), H^{s-m}(\mathbb{R}^d)) \tag{4.13}$$

is continuous.

An operator $\mathrm{Op}^{\mathrm{w}}(a) \in \Psi^m(\mathbb{R}^{2d})$ is *elliptic* if its symbol $a(x, k)$ is elliptic in $S^m(\mathbb{R}^{2d})$. If $a \in \Psi^m$ is elliptic then there exists $b \in \Psi^{-m}$, unique modulo $\Psi^{-\infty}$ such that $ab = ba = \mathbb{1}$ modulo $\Psi^{-\infty}$. Such an operator b is called a *pseudo-inverse* or a *parametrix* of a. We will denote it by $b =: a^{(-1)}$. As a typical example $\mathbb{1} + b$ for $b \in \Psi^{-m}$, $m > 0$ is elliptic in Ψ^0.

The following lemma is proven in [S, Prop. A.1.1, A.1.2] .

Lemma 4.1. *Let $u \in \mathcal{D}'(\mathbb{R}^d)$, $(x, k) \in T^*\mathbb{R}^d\backslash\{0\}$. Then $(x, k) \notin \mathrm{WF}(u)$ iff there exists $\chi \in C_0^\infty(\mathbb{R}^d)$ and $a \in S^0_{\mathrm{ph}}(\mathbb{R}^{2d})$ with $x \in \mathrm{supp}\chi$, $(x, k) \notin \mathrm{Char}(a)$ and $\mathrm{Op}^{\mathrm{w}}(a)\chi u \in \mathcal{S}(\mathbb{R}^d)$.*

4.5. **Functional calculus for pseudo-differential operators.** We now recall various well-known results about functional calculus for pseudo-differential operators.

Proposition 4.2. *Let $a \in \Psi^m(\mathbb{R}^d)$ for $m \geq 0$ be elliptic in $\Psi^m(\mathbb{R}^d)$ and symmetric on $\mathcal{S}(\mathbb{R}^d)$. Then:*

(1) *a is selfadjoint on $H^m(\mathbb{R}^d)$,*
(2) *for $z \notin \sigma(a)$ $(z - a)^{-1} \in \Psi^{-m}(\mathbb{R}^d)$,*
(3) *if $f \in S^p(\mathbb{R})$, $p \in \mathbb{R}$, then $f(a)$, defined by the functional calculus, belongs to $\Psi^{mp}(\mathbb{R}^d)$.*
(4) *if f is elliptic in $S^p(\mathbb{R})$ then $\sigma_{\mathrm{pr}}(f(a)) = f(\sigma_{\mathrm{pr}}(a))$ mod $S^{mp-1}(\mathbb{R}^{2d})$.*
(5) *if $a \in \Psi^m_{\mathrm{ph}}(\mathbb{R}^d)$ and $f \in S^p_{\mathrm{ph}}(\mathbb{R})$, then $f(a) \in \Psi^{mp}_{\mathrm{ph}}(\mathbb{R}^d)$, and if $f \in S^p_{\mathrm{ph}}(\mathbb{R})$ is elliptic, then $\sigma_{\mathrm{pr}}(f(a)) = f_p(\sigma_{\mathrm{pr}}(a))$, where $f_p \in S^p_{\mathrm{h}}(\mathbb{R})$ is the principal symbol of f.*

Proof. We refer the reader for example to [R, Thm. 5.4], [Bo, Corr. 4.5] for the proof of similar statements. Statement (1) follows from the fact that $a + \mathrm{i}\lambda\mathbb{1}$ maps $H^m(\mathbb{R}^d)$ bijectively onto $L^2(\mathbb{R}^d)$ for $|\lambda|$ large enough.

To prove statement (2), the most direct way is to use the Beals criterion (see e.g. [Bo]), which characterizes pseudo-differential operators by properties of the

multi-commutators with the operators x_i, D_j: an operator a belongs to $\Psi^m(\mathbb{R}^d)$ iff:

$$\begin{aligned} & a : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}(\mathbb{R}^d), \\ & \mathrm{ad}_x^\alpha \mathrm{ad}_D^\beta a \in B(H^{m-|\alpha|}(\mathbb{R}^d), L^2(\mathbb{R}^d)), \ \forall\ \alpha, \beta \in \mathbb{N}^d, \end{aligned}$$

where $\mathrm{ad}_{x_i} b = [x_i, b]$, $\mathrm{ad}_{D_j} b = [D_j, b]$, and $\mathrm{ad}_x^\alpha = \mathrm{ad}_{x_1}^{\alpha_1} \cdots \mathrm{ad}_{x_d}^{\alpha_d}$ and similarly for ad_D^β.

From (2) one can deduce (3) by expressing $f(a)$ for $f \in S^p(\mathbb{R})$ using the resolvent $(z-a)^{-1}$ and an almost analytic extension of f, see e.g. [HS, D]. Statement (4) follows from the parametrix construction of $(z-a)^{-1}$, which has $(z - \sigma_{\rm pr}(a))^{-1}$ as principal symbol. Statement (5) can be proved similarly. □

We conclude this subsection by stating a useful lemma, which follows from symbolic calculus.

Lemma 4.3. *Let $a \in \Psi^p(\mathbb{R}^d)$, $p \in \mathbb{R}$, $f, g \in C^\infty(\mathbb{R}^d)$ with $\nabla f, \nabla g \in C_0^\infty(\mathbb{R}^d)$ and $f \equiv 0$ near $\operatorname{supp} g$. Then*

$$f(x) a g(x) \in \Psi^{-\infty}(\mathbb{R}^d).$$

In particular $f(x)ag(x)$ maps $\mathcal{H}'(\mathbb{R}^d)$ into $\mathcal{H}(\mathbb{R}^d)$.

4.6. **Propagators.** Let us fix a map $\epsilon(t) = \epsilon_1(t) + \epsilon_0(t)$, where $\epsilon_i(t) \in C^\infty(\mathbb{R}, \Psi^i(\mathbb{R}^d))$ for $i = 0, 1$. Assume moreover that $\epsilon_1(t)$ is elliptic in $\Psi^1(\mathbb{R}^d)$ and symmetric on $\mathcal{S}(\mathbb{R}^d)$. It follows by Prop. 4.2 that $\epsilon_1(t)$ is selfadjoint with domain $H^1(\mathbb{R}^d)$, hence $\epsilon(t)$ with domain $H^1(\mathbb{R}^d)$ is closed, with non empty resolvent set.

We denote by $\mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma) d\sigma)$ the associated propagator defined by:

$$\begin{cases} \frac{\partial}{\partial t} \mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma) d\sigma) = \mathrm{i}\epsilon(t) \mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma) d\sigma), \\ \frac{\partial}{\partial s} \mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma) d\sigma) = -\mathrm{i} \mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma) d\sigma) \epsilon(s), \\ \mathrm{Texp}(\int_s^s \mathrm{i}\epsilon(\sigma) d\sigma) = \mathbb{1}. \end{cases}$$

Note that the propagator $\mathrm{Texp}(\int_s^t \mathrm{i}\epsilon_1(\sigma) d\sigma)$ exists and is unitary by e.g. [RS, Thm. X.70]. Since $\epsilon(t) - \epsilon_1(t)$ is locally uniformly bounded in $B(L^2(\mathbb{R}^d))$, one easily deduces the existence of $\mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma) d\sigma)$, which is strongly continuous in (t, s) with values in $B(L^2(\mathbb{R}^d))$.

Definition 4.4. *Assume in addition that $\epsilon(t) \in \Psi^1_{\rm ph}(\mathbb{R}^d)$. Then we denote by $\Phi_\epsilon(t, s) : T^*\mathbb{R}^d \backslash \{0\} \to T^*\mathbb{R}^d \backslash \{0\}$ the symplectic flow associated to the time-dependent Hamiltonian $-\sigma_{\rm pr}(\epsilon)(t, x, k)$.*

Equivalently $\Phi_\epsilon(t, s)$ is the restriction to the variables (x, k) of the symplectic flow on $T^*\mathbb{R}^{1+d} \backslash \{0\}$ associated to the Hamiltonian $\tau - \sigma_{\rm pr}(\epsilon)(t, x, k)$.

Clearly $\Phi_\epsilon(t, s)$ is an homogeneous map of degree 0.

The following classical result is known as *Egorov's theorem*, see for instance [T, Sec. 0.9] for the proof.

Proposition 4.5. (1) *$\mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma) d\sigma)$ is bounded on $\mathcal{H}(\mathbb{R}^d)$ hence on $\mathcal{H}'(\mathbb{R}^d)$ by duality.*

(2) *Let $a \in \Psi^m(\mathbb{R}^d)$. Then*

$$a(t, s) := \mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma) d\sigma) a \mathrm{Texp}(\int_t^s \mathrm{i}\epsilon(\sigma) d\sigma)$$

belongs to $C^\infty(\mathbb{R}^2, \Psi^m(\mathbb{R}^d))$. Moreover if $\epsilon(t) \in C^\infty(\mathbb{R}, \Psi^1_{\rm ph}(\mathbb{R}^d))$ and $a \in \Psi^m_{\rm ph}(\mathbb{R}^d)$ then $a(t, s) \in C^\infty(\mathbb{R}^2, \Psi^m_{\rm ph}(\mathbb{R}^d))$ with

$$\sigma_{\rm pr}(a)(t, s) = \sigma_{\rm pr}(a) \circ \Phi_\epsilon(s, t).$$

From Proposition 4.5 and Lemma 4.1 we obtain the following result (the steps of the proof are explained in [T, Sec. 0.10]).

Proposition 4.6. *For $u \in \mathcal{H}'(\mathbb{R}^d)$ one has:*

$$\mathrm{WF}(\mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma)d\sigma)u) = \Phi_\epsilon(t,s)\mathrm{WF}(u),$$

hence

$$\mathrm{WF}(\mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma)d\sigma))' = \{(x,k,x',k') : \ (x,k) = \Phi_\epsilon(t,s)(x',k')\}.$$

Lemma 4.7. *Let $\epsilon(t) \in C^\infty(\mathbb{R}, \Psi^1(\mathbb{R}^d))$ as above, $s_{-\infty}(t,s) \in C^\infty(\mathbb{R}^2, \Psi^{-\infty}(\mathbb{R}^d))$. Then*

$$\mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma)d\sigma)s_{-\infty}(t,s) \in C^\infty(\mathbb{R}^2, \Psi^{-\infty}(\mathbb{R}^d)).$$

Proof. The proof will be given in Subsect. A.1. □

5. Concrete Klein-Gordon equations

5.1. **Model Klein-Gordon equation on $\mathbb{R}^{1+d}$.** In this subsection we describe the model Klein-Gordon equation that will be considered in the sequel. We take $M = \mathbb{R}^{1+d}$, $x = (t, \mathrm{x}) \in \mathbb{R}^{1+d}$ and fix a second order differential operator

$$a(t,\mathrm{x},D_\mathrm{x}) = -\sum_{j,k=1}^d \partial_{\mathrm{x}^j} a^{jk}(x)\partial_{\mathrm{x}^k} + \sum_{j=1}^d b^j(x)\partial_{\mathrm{x}^j} - \partial_{\mathrm{x}^j}\overline{b}^j(x) + m(x), \tag{5.1}$$

where

$$\begin{aligned} &a^{jk}, b^j, m \in C^\infty(\mathbb{R}, C^\infty_{\mathrm{bd}}(\mathbb{R}^d)), \ m(x) \in \mathbb{R}, \\ &[a^{jk}](x) \geq c(t)\mathbb{1} \text{ uniformly on } \mathbb{R}^{1+d}, \ c(t) > 0. \end{aligned} \tag{5.2}$$

We introduce the model Klein-Gordon operator

$$P(x, D_x) = \partial_t^2 + a(t, \mathrm{x}, D_\mathrm{x}),$$

which is formally selfadjoint for the scalar product $(u_1|u_2) = \int_{\mathbb{R}^{1+d}} \overline{u}_1 u_2 dx$.

We will consider the Cauchy problem:

$$\begin{cases} \partial_t^2\phi(t) + a(t,\mathrm{x},D_\mathrm{x})\phi(t) = 0, \\ \phi(s) = f_0, \\ \mathrm{i}^{-1}\partial_t\phi(s) = f_1, \end{cases} \tag{5.3}$$

for $f = (f_0, f_1) \in \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2$. By the well-known method of energy estimates, one obtains the existence and uniqueness of a solution $\phi \in C^\infty(\mathbb{R}, \mathcal{H}(\mathbb{R}^d))$. Similarly if $f \in \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$, there exists a unique solution $\phi \in C^\infty(\mathbb{R}, \mathcal{H}'(\mathbb{R}^d))$.

5.2. **Reduction to the model case.** Consider a globally hyperbolic space-time (M, g) with a Cauchy hypersurface diffeomorphic to $\mathbb{R}^d$. This implies that we can assume that $M = \mathbb{R}_t \times \mathbb{R}^d$ and

$$g = -c(x)dt^2 + h_{jk}(x)d\mathrm{x}^j d\mathrm{x}^k, \tag{5.4}$$

where $x = (t, \mathrm{x})$, $c(x) > 0$ is a smooth function and $h_{jk}(x)d\mathrm{x}^j d\mathrm{x}^k$ is a smooth Riemannian metric on $\mathbb{R}^d$.

In this subsection we explain how to reduce the Klein-Gordon operator (3.4) to the model case considered in Subsect. 5.1.

Writing $A_\mu(x) = (V(x), \mathrm{A}_j(x))$, we have:

$$\begin{aligned} &P(x, D_x) \\ = \ &c^{-\frac12}|h|^{-\frac12}(\partial_t + \mathrm{i}V)c^{-\frac12}|h|^{\frac12}(\partial_t + \mathrm{i}V) \\ &-c^{-\frac12}|h|^{-\frac12}(\partial_j + \mathrm{i}A_j)c^{\frac12}|h|^{\frac12}h^{jk}(\partial_k + \mathrm{i}A_k) + \rho, \end{aligned}$$

where $|h| = \det[h_{jk}]$, $[h^{jk}] = [h_{jk}]^{-1}$.

We choose the Cauchy hypersurface $S = \{0\} \times \mathbb{R}^d$ so that

$$\overline{\phi}_1 \sigma \phi_2 = \int_S \left(\overline{(\partial_t + \mathrm{i}V)\phi_1}\phi_2 - \overline{\phi_1}(\partial_t + \mathrm{i}V)\phi_2 \right) c^{-\frac{1}{2}} |h|^{\frac{1}{2}} d\mathrm{x}. \tag{5.5}$$

Set:

$$\begin{aligned} F(t,\mathrm{x}) = & \int_0^t V(s,\mathrm{x}) ds, \ \tilde{\mathrm{A}} = \mathrm{A} + \nabla F, \ \tilde{\rho} = c\rho - c^{\frac{1}{4}} |h|^{-\frac{1}{4}} \partial_t^2 (c^{-\frac{1}{4}} |h|^{\frac{1}{4}}), \\ a(t,\mathrm{x},D_{\mathrm{x}}) = & \ c^{\frac{1}{4}} |h|^{-\frac{1}{4}} (\partial_j + \mathrm{i}\tilde{\mathrm{A}}_j) c^{\frac{1}{2}} |h|^{\frac{1}{2}} h^{jk} (\partial_k + \mathrm{i}\tilde{\mathrm{A}}_k) c^{\frac{1}{4}} |h|^{-\frac{1}{4}} + \tilde{\rho}. \end{aligned}$$

Lemma 5.1. (1) *Let $b = c^{-\frac{1}{4}} |h|^{\frac{1}{4}}$. Then:*

$$P(x, D_x) = c^{-\frac{1}{2}} |h|^{-\frac{1}{2}} b \mathrm{e}^{-\mathrm{i}F} \left(\partial_t^2 + a(t,\mathrm{x},D_{\mathrm{x}}) \right) b \mathrm{e}^{\mathrm{i}F},$$

hence

$$E = b^{-1} \mathrm{e}^{-\mathrm{i}F} \tilde{E} c^{\frac{1}{2}} |h|^{\frac{1}{2}} b^{-1} \mathrm{e}^{\mathrm{i}F},$$

where $\tilde{E}$ is the Pauli-Jordan function for $\tilde{P}(x, D_x) := \partial_t^2 + a(t,\mathrm{x},D_{\mathrm{x}})$.

(2) *The map:*

$$\phi \mapsto \tilde{\phi} := c^{-\frac{1}{4}} |h|^{\frac{1}{4}} \mathrm{e}^{-\mathrm{i}F} \phi,$$

is symplectic from $(\mathrm{Sol}_{C^\infty}(P), \sigma)$ to $(\mathrm{Sol}_{C^\infty}(\tilde{P}), \tilde{\sigma})$ for

$$\overline{\tilde{\phi}_1} \tilde{\sigma} \tilde{\phi}_2 = \int_S \overline{\partial_t \tilde{\phi}_1} \tilde{\phi}_2 - \overline{\tilde{\phi}_1} \partial_t \tilde{\phi}_2 d\mathrm{x}.$$

(3) *Assume the following hypotheses:*

$$(H) \quad \begin{aligned} & \forall\ I \subset \mathbb{R} \text{ compact interval } \exists\ C > 0 \text{ such that} \\ & C \leq c(x), \ C\mathbb{1} \leq [h_{jk}(x)], \text{ uniformly for } x \in I \times \mathbb{R}^d, \\ & h_{jk}(x), \ c(x), \ \rho(x), A_\mu(x) \in C^\infty(\mathbb{R}, C^\infty_{\mathrm{bd}}(\mathbb{R}^d)). \end{aligned}$$

Then the operator $a(t,\mathrm{x},D_{\mathrm{x}})$ is of the form (5.1) and the conditions (5.2) are satisfied.

Proof. Set

$$b^2 = c^{-\frac{1}{2}} |h|^{\frac{1}{2}}, \ a = (\partial_j + \mathrm{i}A_j) c^{\frac{1}{2}} |h|^{\frac{1}{2}} h^{jk} (\partial_k + \mathrm{i}A_k) + c^{\frac{1}{2}} |h|^{\frac{1}{2}} \rho.$$

Then

$$\begin{aligned} P(x, D_x) = & \ c^{-\frac{1}{2}} |h|^{-\frac{1}{2}} ((\partial_t + \mathrm{i}V) b^2 (\partial_t + \mathrm{i}V) + a), \\ = & \ c^{-\frac{1}{2}} |h|^{-\frac{1}{2}} b ((\partial_t + \mathrm{i}V)^2 + \tilde{a}) b, \end{aligned}$$

for $\tilde{a} = b^{-1} a b^{-1} - b^{-1} (\partial_t^2 b)$. Since $\partial_t + \mathrm{i}V = \mathrm{e}^{-\mathrm{i}F} \partial_t \mathrm{e}^{\mathrm{i}F}$ we finally get:

$$P(x, D_x) = c^{-\frac{1}{2}} |h|^{-\frac{1}{2}} b \mathrm{e}^{-\mathrm{i}F} \left(\partial_t^2 + a(t,\mathrm{x},D_{\mathrm{x}}) \right) \mathrm{e}^{\mathrm{i}F} b,$$

This proves (1). (2) and (3) are left to the reader. □

By Lemma 5.1, the task of constructing Hadamard states for $P(x, D)$ can be reduced to constructing Hadamard states for the model Klein–Gordon equation $\tilde{P}(x, D)$. Indeed, suppose we have a Hadamard state with two-point function $\tilde{\Lambda}$ and charge $\mathrm{i}\tilde{E}$. Then

$$\Lambda := b^{-1} \mathrm{e}^{-\mathrm{i}F} \tilde{\Lambda} c^{\frac{1}{2}} |h|^{\frac{1}{2}} b^{-1} \mathrm{e}^{\mathrm{i}F}$$

defines the two-point function of a Hadamard state with charge $\mathrm{i}E$, the wave front set being preserved by multiplication by smooth densities.

6. The model Klein-Gordon equation

In this section we consider the model Klein-Gordon operator $P(x, D_x) = \partial_t^2 + a(t, \mathrm{x}, D_\mathrm{x})$ introduced in Subsect. 5.1. The associated symplectic form is:

$$\overline{\phi}_1 \sigma \phi_2 = \int_{t \times \mathbb{R}^d} \overline{\partial_t \phi_1} \phi_2 - \overline{\phi_1} \partial_t \phi_2 d\mathrm{x}.$$

6.1. **Notation.** If $a \geq 0$ is a selfadjoint operator on a Hilbert space $\mathfrak{h}$ we write $a > 0$ if $\mathrm{Ker}\, a = \{0\}$. Then a^{-1} with domain $\mathrm{Ran}\, a$ is selfadjoint.

If $a, b \geq 0$ are two selfadjoint operators on a Hilbert space $\mathfrak{h}$ then we write $a \leq b$ if $\mathrm{Dom} b^{\frac{1}{2}} \subset \mathrm{Dom} a^{\frac{1}{2}}$ and $(u|au) \leq (u|bu)$ for $u \in \mathrm{Dom} b^{\frac{1}{2}}$.

The Kato-Heinz theorem says that if $0 \leq a \leq b$ then $0 \leq a^s \leq b^s$ for all $0 \leq s \leq 1$ and if $0 < a \leq b$ then $0 \leq b^{-1} \leq a^{-1}$.

We write $a \sim b$ if $c^{-1} a \leq b \leq ca$ for some $c > 0$.

6.2. **Bicharacteristic curves.** We denote $a_2(t, \mathrm{x}, k) = k_i a^{ij}(t, \mathrm{x}) k_j$ the principal symbol of $a(t, \mathrm{x}, D_\mathrm{x})$ and by $p(x, \xi) = -\tau^2 + a_2(t, \mathrm{x}, k)$ the principal symbol of $P(x, D_x) = \partial_t^2 + a(t, \mathrm{x}, D_\mathrm{x})$.

We set:

$$\epsilon_1(t, \mathrm{x}, k) = (k_i a^{ij}(t, \mathrm{x}) k_j)^{\frac{1}{2}}.$$

As in Def. 4.4 we denote by $\Phi_\pm(t, s) : T^*\mathbb{R}^d \backslash \{0\} \to T^*\mathbb{R}^d \backslash \{0\}$ the restrictions to the variables (x, k) of the symplectic flows on $T^*\mathbb{R}^{1+d} \backslash \{0\}$ associated to the hamiltonians $\tau \mp \epsilon_1(t, \mathrm{x}, k)$.

The following lemma is immediate:

Lemma 6.1. *Let $X_i \in \mathcal{N}_\pm$, $i = 1, 2$ with $X_1 \sim X_2$. Then*

$$X_i = (t_i, \mathrm{x}_i, \pm\epsilon_1(t_i, \mathrm{x}_i, k_i), k_i) \text{ with } (\mathrm{x}_2, k_2) = \Phi_\pm(t_2, t_1)(\mathrm{x}_1, k_1).$$

6.3. **Parametrix for the Cauchy problem.** In this subsection we outline the well-known construction of a parametrix for the Cauchy problem (5.3). The construction is well-known and belongs to the folklore of microlocal analysis. Usually it is done using Fourier integral operators. Our construction relies more on Hilbert space methods.

We start by an auxiliary lemma.

Lemma 6.2. *Assume (5.2) and let $a(t, \mathrm{x}, D_\mathrm{x})$ be given by (5.1). Then there exists smooth maps*

$$\begin{aligned} \mathbb{R} \ni t &\mapsto \epsilon(t) = \epsilon(t, \mathrm{x}, k) \in S^1_{\mathrm{ph}}(\mathbb{R}^{2d}), \\ \mathbb{R} \ni t &\mapsto r_{-\infty}(t) = r_{-\infty}(t, \mathrm{x}, k) \in S^{-\infty}(\mathbb{R}^{2d}), \end{aligned}$$

such that:

(1) *$\epsilon(t, \mathrm{x}, k)$ is real-valued, $\epsilon(t, \mathrm{x}, k) \in C^\infty(\mathbb{R}, S^1_{\mathrm{ph}}(\mathbb{R}^{2d}))$ with principal symbol*

$$\epsilon_1(t, \mathrm{x}, k) = (k_i a^{ij}(t, \mathrm{x}) k_j)^{\frac{1}{2}},$$

(2) *$\epsilon^\mathrm{w}(t, \mathrm{x}, D_\mathrm{x}) \geq c(t)(D_x^2 + \mathbb{1})^{\frac{1}{2}}$ for $c(t) > 0$,*

(3) *$a(t, \mathrm{x}, D_\mathrm{x}) = \epsilon^\mathrm{w}(t, \mathrm{x}, D_\mathrm{x})^2 - r^\mathrm{w}_{-\infty}(t, \mathrm{x}, D_\mathrm{x})$.*

Moreover $\epsilon(t)$ and $r_{-\infty}(t)$ are unique modulo $C^\infty(\mathbb{R}, \Psi^{-\infty}(\mathbb{R}^d))$.

Proof. The proof will be given in Subsect. A.2. □

The following theorem is the main result of this section. It will be used later on to characterize and construct examples of quasi-free Hadamard states.

Theorem 6.3. *There exist operators* $b(t) \in C^\infty(\mathbb{R}, \Psi^1_{\rm ph}(\mathbb{R}^d))$, $r(t) \in C^\infty(\mathbb{R}, \Psi^{-1}_{\rm ph}(\mathbb{R}^d))$ *with*

$$\begin{array}{rl} (i) & b(t) = \epsilon(t) + (2\epsilon(t))^{-1}{\rm i}\partial_t\epsilon(t) \ \ mod\ C^\infty(\mathbb{R}, \Psi^{-1}(\mathbb{R}^d)),\\ (ii) & r(t) = b^*(t)^{(-1)} \ \ mod\ C^\infty(\mathbb{R}, \Psi^{-\infty}(\mathbb{R}^d)),\\ (iii) & r(t) = \epsilon(t)^{-1} + C^\infty(\mathbb{R}, \Psi^{-2}(\mathbb{R}^d)),\\ (iv) & r(t) + r(t)^* \sim \epsilon(t)^{-1}, \end{array}$$

such that if

$$\begin{array}{rl} u_+(t,s) := & {\rm Texp}({\rm i}\int_s^t b(\sigma)d\sigma),\ \ u_-(t,s) := {\rm Texp}(-{\rm i}\int_s^t b^*(\sigma)d\sigma)\\ d_+(t) := & (\mathbb{1} + b^*(t)^{(-1)}b(t))^{(-1)},\ \ d_-(t) := d_+(t)^*,\\ r_+(t) := & r(t),\ \ r_-(t) := r^*(t), \end{array}$$

the following properties hold:

(1) *set for* $f \in \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$*:*

$$\begin{array}{rl} U(t,s)f = & u_+(t,s)d_+(s)\left(f_0 + r_+(s)f_1\right) + u_-(t,s)d_-(s)\left(f_0 - r_-(s)f_1\right),\\ =: & U_+(t,s)f + U_-(t,s)f. \end{array}$$

then

$$\left\{\begin{array}{l} (\partial_t^2 + a(t,{\rm x},D_{\rm x}))U(t,s)f = s_{-\infty}(t,s)f,\\ U(s,s)f = f_0 + r_{-\infty,0}(s)f,\\ {\rm i}^{-1}\partial_t U(t,s)f|_{t=s} = f_1 + r_{-\infty,1}(s)f, \end{array}\right. \tag{6.1}$$

for $s_{-\infty}(t,s) \in C^\infty(\mathbb{R}^2, \Psi^{-\infty}(\mathbb{R}^d)) \otimes \mathbb{C}^2$, $r_{-\infty,i}(s) \in C^\infty(\mathbb{R}, \Psi^{-\infty}(\mathbb{R}^d)) \otimes \mathbb{C}^2$.

(2) *let* $\phi(t)$ *be the unique solution of (5.3) for* $f \in \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$*. Then:*

$$\phi(t) = U(t,s)f \ \text{mod}\ C^\infty(\mathbb{R}, \mathcal{H}(\mathbb{R}^d)). \tag{6.2}$$

Proof. the proof will be given in Subsect. A.3. □

To simplify notation, in the rest of the paper, we will fix $s = 0$, and set:

$$\begin{array}{l} b := b(0),\ \ u_\pm(t) := u_\pm(t,0),\ \ U(t) := U(t,0),\\ d := d(0),\ \ r := r(0),\ \ \epsilon := \epsilon(0). \end{array}$$

The constructions of Hadamard states in Sect. 7 will a priori depend on the choice of an operator r. To study this dependence it is convenient to introduce the following definition.

Definition 6.4. *We denote by* $\mathcal{M}$ *the set:*

$$\mathcal{M} := \{r \in \Psi^{-1}_{\rm ph}(\mathbb{R}^d)\ :\ r = b^{*(-1)} + \Psi^{-\infty}(\mathbb{R}^d),\ r + r^* \sim \epsilon^{-1}\}.$$

Remark 6.5. *Note that the operator* b *in Thm. 6.3 is unique modulo* $\Psi^{-\infty}$*. Thm. 6.3 implies that* $\mathcal{M}$ *is not empty. Since two elements of* $\mathcal{M}$ *are equal modulo* $\Psi^{-\infty}$*, the conclusions of Thm. 6.3 are valid for any* $r \in \mathcal{M}$*.*

The following corollary is a consequence of (6.2), Prop. 4.6 and Lemma 6.1.

Corollary 6.6. *If* $\phi(t)$ *is the unique solution of (5.3) for* $f \in \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$*, one has*

$$\phi(t) = U_+(t)f + U_-(t)f \ \text{mod}\ C^\infty(\mathbb{R}, \mathcal{H}(\mathbb{R}^d)),$$

and

$$\begin{array}{rl} & {\rm WF}(U_\pm(t)f)\\ = & \{(x_2,\xi_2) :\ \exists\ ({\rm x}_1,k_1) \in {\rm WF}(f_0 \pm r_\pm f_1)\ \textit{with}\ (s,{\rm x}_1,\pm\epsilon({\rm x}_1,k_1),k_1) \sim (x_2,\xi_2)\}. \end{array}$$

In particular

$$\mathrm{WF}(U_\pm(t)f) \subset \mathcal{N}_\pm.$$

6.4. **Symplectic properties of the spaces of positive/negative wavefront set solutions.** We now investigate the properties, with respect to the symplectic form σ, of the spaces of solutions of the Klein-Gordon equation having wavefront set included in the positive/negative energy surfaces $\mathcal{N}_\pm$.

Of course we cannot work with solutions in $\mathcal{E}(M)$, since their wavefront set is empty, nor with solutions in $\mathcal{D}'(M)$, since the symplectic form σ is not defined on arbitrary distributional solutions. A natural space of solutions is the space of *finite energy solutions* defined as follows:

$$\mathrm{Sol}_E(P) := \{\phi \in C^0(\mathbb{R}, H^1(\mathbb{R}^d)) \cap C^1(\mathbb{R}, L^2(\mathbb{R}^d)) \ : \ P(t, \mathrm{x}, D_\mathrm{x})\phi = 0\}.$$

It is well-known that $\phi \in \mathrm{Sol}_E(P)$ iff $f = (\phi(0), \mathrm{i}^{-1}\partial_t\phi(0)) \in H^1(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$. Moreover the symplectic form σ is well defined in $\mathrm{Sol}_E(P)$.

Recall that for $r \in \mathcal{M}$ one sets $r_+ = r, \ r_- = r^*$. We define now

$$C^\pm(r) := \{f \in H^1(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d) \ : \ f_0 \mp r_\mp f_1 = 0\},$$

and

$$\mathrm{Sol}_E^\pm(P, r) := \{\phi \in \mathrm{Sol}_E(P) \ : \ (\phi(0); \mathrm{i}^{-1}\partial_t\phi(0)) \in C^\pm(r)\}.$$

We call $\mathrm{Sol}_E^\pm(P, r)$ the space of *positive/negative wavefront set solutions.*

Theorem 6.7. *Let $r \in \mathcal{M}$. Then the following properties hold:*
1. $\mathrm{Sol}_E(P) = \mathrm{Sol}_E^+(P, r) \oplus \mathrm{Sol}_E^-(P, r)$,
2. $\phi \in \mathrm{Sol}_E^\pm(P, r) \ \Rightarrow \ \mathrm{WF}(\phi) \subset \mathcal{N}_\pm$,
3. $\pm\mathrm{i}\sigma = \pm q > 0$ *on* $\mathrm{Sol}_E^\pm(P, r)$,
4. *the spaces* $\mathrm{Sol}_E^\pm(P, r)$ *are symplectically orthogonal.*

Remark 6.8. *We can interpret Thm. 6.7 as follows: the space of finite energy solutions decomposes as the direct sum of the spaces of positive resp. negative wavefront set solutions. The charge q is positive, resp. negative on these spaces. Moreover these two spaces are symplectically orthogonal. This is the exact analogue of the well-known situation in the static case, where $a(t, \mathrm{x}, D_\mathrm{x})$ does not depend on t (cf. Subsect. 7.5).*

For the proof of Thm. 6.7, we will use the following lemma.

Lemma 6.9. *Let $r \in \mathcal{M}$. Then:*
1. $r + r^* : H^1(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ *is invertible and*
$$(r + r^*)^{-\frac{1}{2}} = \frac{1}{\sqrt{2}}\epsilon^{\frac{1}{2}} + \Psi^0_{\mathrm{ph}}(\mathbb{R}^d).$$
2. *The operator*
$$T(r) := (r + r^*)^{-\frac{1}{2}} \begin{pmatrix} \mathbb{1} & r \\ \mathbb{1} & -r^* \end{pmatrix} : \ \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2,$$
is bounded with bounded inverse:
$$T(r)^{-1} = \begin{pmatrix} r^* & r \\ \mathbb{1} & -\mathbb{1} \end{pmatrix} (r + r^*)^{-\frac{1}{2}}.$$
3. $T(r) : H^1(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d) \to H^{\frac{1}{2}}(\mathbb{R}^d) \otimes \mathbb{C}^2$ *is bounded with inverse* $T(r)^{-1}$.
4. *one has:*
$$\tilde{q} := (T(r)^{-1})^* \circ q \circ T(r)^{-1} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}.$$

Proof. From Thm. 6.3 we obtain that $r + r^* \sim \epsilon^{-1}$, which implies that $r + r^*$ is bijective from $H^1(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$. Moreover $(r+r^*)^{-1} = \frac{1}{2}\epsilon + \Psi^0$ and $(r+r^*)^{-1} \sim \epsilon$. By Prop. 4.2 we obtain (1). Statements (2), (3), (4) follow from (1). $\square$

Proof of Thm. 6.7. For $\tilde{f} \in H^{\frac{1}{2}}(\mathbb{R}^d) \otimes \mathbb{C}^2$ we set $\tilde{f} = (\tilde{f}_+, \tilde{f}_-)$. Since $r_+ = r$, $r_- = r^*$ we obtain that by Lemma 6.9 $f \in C^\pm$ iff $(Tf)_\mp = 0$. The theorem follows then from Lemma 6.9 (4). $\square$

7. Construction of Hadamard states

7.1. **Microlocal spectrum condition.** In this subsection we discuss conditions under which a covariance c on $\mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2$ leads by(3.6) to a covariance C on $\mathcal{D}(M)$ satisfying the microlocal spectrum condition in Def. 3.2.

Recall that $c : E_1 \to E_2$ means that c is linear continuous between the two topological vector spaces E_1 and E_2.

We consider the model Klein-Gordon equation:

$$\partial_t^2 \phi + a(t, \mathrm{x}, D_\mathrm{x})\phi = 0,$$

introduced in Subsect. 5.1.

Let c be a bounded hermitian form on $\mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2$. We identify it with the operator:

$$c = \begin{pmatrix} c_{00} & c_{01} \\ c_{10} & c_{11} \end{pmatrix} : \ \mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{D}'(\mathbb{R}^d) \otimes \mathbb{C}^2, \tag{7.1}$$

and associate to it the bounded hermitian form C on $\mathcal{D}(\mathbb{R}^{1+d})$ given by:

$$(u|Cv) = (\rho \circ Eu | c\rho \circ Ev), \ C : \mathcal{D}(\mathbb{R}^{1+d}) \to \mathcal{D}'(\mathbb{R}^{1+d}). \tag{7.2}$$

We still denote by $C \in \mathcal{D}'(\mathbb{R}^{1+d} \times \mathbb{R}^{1+d})$ the distribution kernel of C given by:

$$(u|Cv) = \int C(x, y)\overline{u}(x)v(y)dxdy.$$

We fix now an operator $r \in \mathcal{M}$ (see Def. 6.4). The map $T(r)$ in Lemma 6.9 will be denoted by T for simplicity.

We would like to define:

$$\tilde{c} := (T^{-1})^* \circ c \circ T^{-1} =: \begin{pmatrix} \tilde{c}_{++} & \tilde{c}_{+-} \\ \tilde{c}_{-+} & \tilde{c}_{--} \end{pmatrix}. \tag{7.3}$$

Since T, $T^{-1} : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$, a natural requirement is that

$$c : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2,$$

which implies that $c : \mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{D}'(\mathbb{R}^d) \otimes \mathbb{C}^2$. In the next theorem we will need to impose stronger conditions on c.

We can now state the main result of this subsection. Recall that the notations ${}_M\Gamma$ and Γ_M for a conic set Γ are defined in Subsect. 3.2.

Theorem 7.1. *Assume that*

$$(1a) \ c : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2,$$

$$(1b) \ {}_{\mathbb{R}^d}\mathrm{WF}(c)' = \mathrm{WF}(c)'_{\mathbb{R}^d} = \emptyset.$$

Then C defined by (7.2) satisfies the microlocal spectrum condition iff:

$$(2) \ \mathrm{WF}(\tilde{c}_{--})' = \mathrm{WF}(\tilde{c}_{+-})' = \mathrm{WF}(\tilde{c}_{-+})' = \emptyset, \ \mathrm{WF}(\tilde{c}_{++})' \subset \Delta,$$

where Δ is the diagonal in $T^*\mathbb{R}^d \backslash \{0\} \times T^*\mathbb{R}^d \backslash \{0\}$.

Remark 7.2. *Note that condition (2) implies that condition (1b) is satisfied by* $\tilde{c}$. *Using that* T, T^{-1} *are pseudo-differential operators, it is easy to see that condition (1b) is then also satisfied by* c. *Therefore if conditions (1a), (2) are satisfied,* C *satisfies* (μsc).

Remark 7.3. *Note that we strengthen the assumption on the sesquilinear form* c, *since we require in (1a) that* $c : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2$ *instead of* $c : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$ *as before. In fact since the Cauchy surface is not compact, some care is needed with the composition of operators.*

Condition (1b) is satisfied for example if $\mathrm{WF}(c)' \subset \Gamma$, *where* Γ *is the graph of a conic, bijective map on* $T^*\mathbb{R}^d$. *This is the case if the entries of* c *are pseudo-differential or even Fourier integral operators.*

Proof.

We set

$$\tilde{\rho} = T \circ \rho =: \tilde{\rho}_+ \oplus \tilde{\rho}_-,$$

so that:

$$C = (\tilde{\rho} \circ E)^* \circ \tilde{c} \circ (\tilde{\rho} \circ E) = \sum_{\alpha,\beta \in \{+,-\}} C_{\alpha\beta}, \tag{7.4}$$

for

$$C_{\alpha\beta} := (\tilde{\rho}_\alpha \circ E)^* \circ \tilde{c}_{\alpha\beta} \circ (\tilde{\rho}_\beta \circ E). \tag{7.5}$$

Let us first check that we can perform the various compositions in (7.4).

Because of the well-known support properties of $E_\pm$ we have:

$$\begin{aligned} \rho \circ E : \quad & \begin{array}{l} \mathcal{D}(M) \to \mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2, \\ \mathcal{E}'(M) \to \mathcal{E}'(\mathbb{R}^d) \otimes \mathbb{C}^2, \end{array} \\ (\rho \circ E)^* : \quad & \begin{array}{l} \mathcal{D}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{D}'(M), \\ \mathcal{E}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{E}(M). \end{array} \end{aligned} \tag{7.6}$$

Note also that $T : \mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2$ and $T : \mathcal{E}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$. We obtain that

$$\begin{aligned} \tilde{\rho} \circ E : \quad & \begin{array}{l} \mathcal{D}(M) \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, \\ \mathcal{E}'(M) \to \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2, \end{array} \\ (\tilde{\rho} \circ E)^* : \quad & \begin{array}{l} \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{D}'(M), \\ \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{E}(M). \end{array} \end{aligned} \tag{7.7}$$

Since we assumed that $c : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$, we have $\tilde{c} : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$, using that T, T^{-1} preserve $\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2$ and $\mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2$. Therefore we can perform the compositions in (7.4).

By Lemma 3.1, we have

$$\mathrm{WF}(E)' = \{(X_1, X_2) : \ X_1 \sim X_2, \ X_1, X_2 \in \mathcal{N}\},$$

and using that the Cauchy surface $\{t = 0\}$ is non-characteristic for the Klein-Gordon equation, we have for $i = 0, 1$:

$$\begin{aligned} & \mathrm{WF}(\rho_i \circ E)' \\ = \ & \{((\mathrm{x}_1, k_1), (x_2, \xi_2)) \in T^*(\mathbb{R}^d \times M) \backslash Z : \ (0, \mathrm{x}_1, -\epsilon_1(0, \mathrm{x}_1, k_1), k_1) \sim (x_2, \xi_2)\} \\ \cup \ & \{((\mathrm{x}_1, k_1), (x_2, \xi_2)) \in T^*(\mathbb{R}^d \times M) \backslash Z : \ (0, \mathrm{x}_1, +\epsilon_1(0, \mathrm{x}_1, k_1), k_1) \sim (x_2, \xi_2)\}. \end{aligned}$$

Then from Corollary 6.6, we obtain that:

$$\mathrm{WF}(\tilde{\rho}_\pm \circ E)' = \Gamma_\pm, \tag{7.8}$$

for

$$\Gamma_\pm = \{((\mathrm{x}_1, k_1), (x_2, \xi_2)) \in T^*(\mathbb{R}^d \times M)\backslash Z : \ (0, \mathrm{x}_1, \pm\epsilon(0, \mathrm{x}_1, k_1), k_1) \sim (x_2, \xi_2)\}.$$

We also have

$$\mathrm{WF}((\tilde{\rho}_\pm \circ E)^*)' = \mathrm{Exch}(\Gamma_\pm). \tag{7.9}$$

We now want to apply the composition rule for the wave front set recalled in Subsect. 3.2 to the identity (7.5), in order to bound $\mathrm{WF}(C_{\alpha\beta})'$. It clearly suffices to bound $\mathrm{WF}(\chi C_{\alpha\beta}\chi)'$ for $\chi \in C_0^\infty(M)$.

Step 1. The first step is to reduce oneself to the composition of properly supported kernels, modulo smoothing operators.

Because of the support properties of the kernel of E, there exists $\psi \in C_0^\infty(\mathbb{R}^d)$ such that (denoting again $\begin{pmatrix} \psi & 0 \\ 0 & \psi \end{pmatrix}$ by ψ):

$$\rho \circ E\chi = \psi\rho \circ E\chi.$$

Let us also fix $\psi_1 \in C_0^\infty(\mathbb{R}^d)$ with $\psi_1 \equiv 1$ near $\mathrm{supp}\psi$. By Lemma 4.3 we know that $(1-\psi_1)T\psi \in \Psi^{-\infty}(\mathbb{R}^d)$, hence

$$\tilde{\rho} \circ E\chi = \psi_1\tilde{\rho} \circ E\chi + R_1\rho \circ E\chi,$$

for

$$R_1 := (1-\psi_1)T\psi : \mathcal{D}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2. \tag{7.10}$$

Taking adjoints we have:

$$\begin{aligned} &\chi(\tilde{\rho} \circ E)^* = (\tilde{\rho} \circ E\chi)^* = \chi(\tilde{\rho} \circ E)^*\psi_1 + \chi(\rho \circ E)^* R_1^*, \\ &R_1^* : \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2. \end{aligned}$$

It follows that

$$\begin{aligned} & \chi(\tilde{\rho} \circ E)^*\tilde{c}(\tilde{\rho} \circ E)\chi \\ = \ & \chi(\tilde{\rho} \circ E)^*\psi_1\tilde{c}\psi_1(\tilde{\rho} \circ E)\chi + \chi(\tilde{\rho} \circ E)^*\tilde{c}R_1(\rho \circ E)\chi + \chi(\tilde{\rho} \circ E)^* R_1^*\tilde{c}\psi_1(\tilde{\rho} \circ E)\chi \\ =: \ & \chi(\tilde{\rho} \circ E)^*\psi_1\tilde{c}\psi_1(\tilde{\rho} \circ E)\chi + I_1 + I_2. \end{aligned}$$

We claim that

$$I_1, \ I_2 : \mathcal{D}'(M) \to \mathcal{D}(M). \tag{7.11}$$

Note that from hypothesis (1a) and the fact that T, T^{-1} are (matrices of) pseudo-differential operators, we know that $\tilde{c} : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2$.

Using then (7.6), (7.7), (7.10) we have:

$$\begin{aligned} I_1 : \quad & \mathcal{D}'(M) : \xrightarrow{(\rho\circ E)\chi} \mathcal{E}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \subset \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \xrightarrow{R_1} \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \\ & \xrightarrow{\tilde{c}} \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \subset \mathcal{E}(\mathbb{R}^d) \otimes \mathbb{C}^2 \xrightarrow{\chi(\tilde{\rho}\circ E)^*} \mathcal{D}(M), \end{aligned}$$

and:

$$\begin{aligned} I_2 : \quad & \mathcal{D}'(M) : \xrightarrow{(\tilde{\rho}\circ E)\chi} \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \xrightarrow{\tilde{c}\psi_1} \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \\ & \xrightarrow{R_1^*} \mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2 \subset \mathcal{E}(\mathbb{R}^d) \otimes \mathbb{C}^2 \xrightarrow{\chi(\rho\circ E)^*} \mathcal{D}(M), \end{aligned}$$

which proves (7.11). It follows that if $\psi_2 \in C_0^\infty(\mathbb{R}^d)$ with $\psi_2 \equiv 1$ near $\mathrm{supp}\psi_1$ we have:

$$\chi C_{\alpha\beta}\chi = \chi(\tilde{\rho}_\alpha \circ E)^*\psi_1 \circ \psi_2\tilde{c}\psi_2 \circ \psi_1(\tilde{\rho}_\beta \circ E)\chi \bmod C^\infty(M \times M),$$

the three operators in the composition above having compactly (hence properly) supported kernels.

Step 2. We check that we can apply the composition rule for wave front sets. Note first that since T, T^{-1} are (matrices of) pseudo-differential operators, we obtain using hypothesis (1b) that:

$$ {}_{\mathbb{R}^d}\mathrm{WF}(\tilde{c})' = \mathrm{WF}(\tilde{c})'_{\mathbb{R}^d} = \emptyset. \tag{7.12}$$

Let us fix $\alpha, \beta \in \{+,-\}$ and set:

$$K_\alpha = \chi(\tilde{\rho}_\alpha \circ E)^* \psi_1, \ K_{\alpha\beta} = \psi_2 \tilde{c}_{\alpha\beta}\psi_2, \ K_\beta = \psi_1(\tilde{\rho}_\beta \circ E)\chi.$$

Using (7.8), (7.9) we have:

$$\mathrm{WF}(K_\alpha)' \subset \mathrm{Exch}(\Gamma_\alpha), \ \mathrm{WF}(K_{\alpha\beta})' \subset \mathrm{WF}(\tilde{c}_{\alpha\beta})', \ \mathrm{WF}(K_\beta)' \subset \Gamma_\beta.$$

It follows also from (7.12) that:

$$\begin{aligned} &{}_M\mathrm{WF}(K_\alpha)' = \mathrm{WF}(K_\alpha)'_{\mathbb{R}^d} = {}_{\mathbb{R}^d}\mathrm{WF}(K_{\alpha\beta})' \\ &= \mathrm{WF}(K_{\alpha\beta})'_{\mathbb{R}^d} = {}_{\mathbb{R}^d}\mathrm{WF}(K_{\alpha\beta})' = \mathrm{WF}(K_\beta)'_M = \emptyset. \end{aligned}$$

It follows that we can compose $K_{\alpha\beta}$ and K_β and

$$\mathrm{WF}(K_{\alpha\beta} \circ K_\beta)' \subset \mathrm{WF}(\tilde{c}_{\alpha\beta}) \circ \Gamma_\beta.$$

We can also compose K_α and $K_{\alpha\beta} \circ K_\beta$ and

$$\mathrm{WF}(K_\alpha \circ K_{\alpha\beta} \circ K_\beta) \subset \mathrm{Exch}(\Gamma_\alpha) \circ \mathrm{WF}(\tilde{c}_{\alpha\beta}) \circ \Gamma_\beta.$$

Step 3. Recalling the definition of Γ_α, Γ_β, we obtain from Step 2 that:

$$\begin{aligned} &\mathrm{WF}(C_{\alpha\beta})' \\ \subset \ &\{(x_1,\xi_1,x_2,\xi_2) \ : \ (x_1,\xi_1) \in \mathcal{N}_\alpha, \ (x_2,\xi_2) \in \mathcal{N}_\beta, \ \exists\ (\mathrm{x}_1,k_1,\mathrm{x}_2,k_2) \in \mathrm{WF}(\tilde{c}_{\alpha\beta})' \\ &\text{such that } (x_1,\xi_1) \sim (0,\mathrm{x}_1,\alpha\epsilon(0,\mathrm{x}_1,k_1),k_1), \ (x_2,\xi_2) \sim (0,\mathrm{x}_2,\beta\epsilon(0,\mathrm{x}_2,k_2))\}. \end{aligned} \tag{7.13}$$

Let $S_{\alpha\beta}$ be the set in the r.h.s. of (7.13). Using (7.4) and the fact that the $S_{\alpha\beta}$ are pairwise disjoint, we obtain that:

$$\mathrm{WF}(C)' \subset \bigcup_{\alpha,\beta\in\{+,-\}} S_{\alpha\beta}.$$

Therefore C satisfies the microlocal spectrum condition iff

$$\begin{aligned} S_{\alpha\beta} = \ &\emptyset, \text{ for } (\alpha,\beta) \neq (+,+), \\ S_{++} \subset \ &\{(x_1,\xi_1,x_2,\xi_2) \ : \ (x_i,\xi_i) \in \mathcal{N}_+, \ (x_1,\xi_1) \sim (x_2,\xi_2)\}. \end{aligned}$$

This condition is satisfied iff

$$\mathrm{WF}(\tilde{c}_{\alpha\beta})' = \emptyset \text{ for } (\alpha,\beta) \neq (+,+), \ \mathrm{WF}(\tilde{c}_{++})' \subset \Delta.$$

This completes the proof of the theorem. □

7.2. **Construction of Hadamard states.** In this subsection we construct a large class of two-point functions λ with pseudo-differential entries, such that Λ is the two-point function of a (gauge-invariant) quasi-free Hadamard state. Beside the microlocal condition in Thm. 7.1, λ should also satisfy the positivity conditions recalled in Subsect. 2.2, i.e. $\lambda \geq 0$, $\lambda \geq q$, where $q = \mathrm{i}\sigma = \left(\begin{smallmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{smallmatrix}\right)$.

As before we fix $r \in \mathcal{M}$.

Proposition 7.4. *Let λ be a two-point function with pseudo-differential entries. Let $\tilde{\lambda}_{\alpha\beta}$ for $\alpha, \beta \in \{+,-\}$ be defined as in (7.3). Then λ is a Hadamard charge density iff*

$$(\mu\mathrm{sc}')\ \tilde{\lambda}_{--},\ \tilde{\lambda}_{+-}, \tilde{\lambda}_{-+} \in \Psi^{-\infty}(\mathbb{R}^d),$$

$$(1)\ \tilde{\lambda}_{++} \geq 1\!\!1,\ \textit{on } \mathcal{H}(\mathbb{R}^d),\ \tilde{\lambda}_{--} \geq 0 \textit{ on } \mathcal{H}(\mathbb{R}^d),$$

$$(2)\ |(u|\tilde{\lambda}_{+-}v)| \leq (u|\tilde{\lambda}_{++}u)^{\frac{1}{2}}(v|\tilde{\lambda}_{--}v)^{\frac{1}{2}},\ u,v \in \mathcal{H}(\mathbb{R}^d),$$

$$(3)\ |(u|\tilde{\lambda}_{+-}v)| \leq (u|(\tilde{\lambda}_{++} - 1\!\!1)u)^{\frac{1}{2}}(v|(\tilde{\lambda}_{--} + 1\!\!1)v)^{\frac{1}{2}},\ u,v \in \mathcal{H}(\mathbb{R}^d).$$

Proof. Since the entries of λ, $\tilde{\lambda}$ are pseudo-differential operators, condition (1a) of Thm. 7.1 is satisfied and condition (1b) as well by Remark 7.2. Moreover, condition (μsc$'$) is equivalent to (2) of Thm. 7.1, hence (μsc$'$) is equivalent to the microlocal spectrum condition.

From Sect. 2 we know that λ is the two-point function of a gauge-invariant quasi-free state iff

$$\lambda \geq 0,\ \lambda \geq q \ \text{ on } \mathcal{D}(\mathbb{R}^d) \otimes \mathbb{C}^2 \Leftrightarrow \lambda \geq 0,\ \lambda \geq q \ \text{ on } \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, \tag{7.14}$$

using that the entries of λ are pseudo-differential operators.

We recall that $\tilde{\lambda} = (T^{-1})^* \circ \lambda \circ T^{-1}$ and $\tilde{q} = (T^{-1})^* \circ q \circ T^{-1}$. By Lemma 6.9 we have

$$\tilde{q} = \begin{pmatrix} 1\!\!1 & 0 \\ 0 & -1\!\!1 \end{pmatrix} :\ \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2.$$

Since T maps $\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2$ into itself bijectively, (7.14) is equivalent to:

$$\tilde{\lambda} \geq 0,\ \tilde{\lambda} \geq \tilde{q} \ \text{ on } \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2. \tag{7.15}$$

Clearly if a, b, c are linear operators with domain $\mathcal{H}(\mathbb{R}^d)$ one has:

$$\begin{aligned} & 2\mathrm{Re}(u|bv) + (u|au) + (v|cv) \geq 0,\ u,v \in \mathcal{H}(\mathbb{R}^d) \\ \Leftrightarrow\quad & |(u|bv)| \leq (u|au)^{\frac{1}{2}}(v|cv)^{\frac{1}{2}},\ u,v \in \mathcal{H}(\mathbb{R}^d) \text{ and } a,c \geq 0 \text{ on } \mathcal{H}(\mathbb{R}^d). \end{aligned}$$

Applying this observation and noting that $r + r^* \geq 0$, we obtain that condition (7.15) is equivalent to conditions (1), (2), (3). □

We now proceed to construct a large class of pseudo-differential operators $\tilde{\lambda}_{\alpha\beta}$ satisfying the conditions in Prop. 7.4.

Theorem 7.5. *Let us fix pseudo-differential operators:*

$$a_{-\infty} \in \Psi^{-\infty}(\mathbb{R}^d),\ a_0 \in \Psi^0(\mathbb{R}^d) \textit{ with } \|a_0\| \leq 1,\ b \in \Psi^{\infty}(\mathbb{R}^d),$$

and set:

$$\begin{aligned} \tilde{\lambda}_{++} &= 1\!\!1 + b^* b, \\ \tilde{\lambda}_{--} &= a^*_{-\infty} a_{-\infty}, \\ \tilde{\lambda}_{+-} &= \tilde{\lambda}^*_{-+} = b^* a_0 a_{-\infty}. \end{aligned}$$

Then the two-point function λ given by (7.3) is the two-point function of a Hadamard state.

Proof. We check the conditions in Prop. 7.4. Conditions (μsc) and (1) are clearly satisfied. From the form of $\tilde{\lambda}_{+-}$ we have

$$|(u|\tilde{\lambda}_{+-}v)| \leq (u|b^* bu)^{\frac{1}{2}}(v|a^*_{-\infty} a_{-\infty} v)^{\frac{1}{2}},\ u,v \in \mathcal{H}(\mathbb{R}^d),$$

which implies (2) and (3), using the form of $\tilde{\lambda}_{++}$ and $\tilde{\lambda}_{--}$. □

7.3. **Symplectic transformations.** Recall from Sect. 2 that if $(\mathcal{Y}, \sigma)$ is a complex symplectic space and $q = \mathrm{i}\sigma$, then the set of two-point functions of gauge-invariant quasi-free states is invariant under conjugation by elements of $U(\mathcal{Y}, q)$. The same is true for the set of two-point functions of pure quasi-free states.

In this subsection we describe a class of symplectic transformations $u \in U(\mathcal{D}(\mathbb{R}^d)\otimes \mathbb{C}^2, q)$ which preserve the microlocal spectrum condition (μsc). We start with a general result.

Proposition 7.6. *Let u such that $u, u^* : \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2$. Set*

$$\tilde{u} := TuT^{-1} = \begin{pmatrix} \tilde{u}_{++} & \tilde{u}_{+-} \\ \tilde{u}_{-+} & \tilde{u}_{--} \end{pmatrix},$$

and assume that

$$\mathrm{WF}(\tilde{u}^*_{++}\tilde{\lambda}_{++}\tilde{u}_{++})' \subset \Delta, \ \tilde{u}_{+-} : \mathcal{H}'(\mathbb{R}^d) \to \mathcal{H}(\mathbb{R}^d).$$

Then if λ is a two-point function with pseudo-differential entries satisfying (μsc), the two-point function $u^*\lambda u$ satisfies also (μsc).

Proof. We set $c := u^*\lambda u$ and as in Subsect. 7.1:

$$\tilde{\lambda} := (T^{-1})^*\lambda T^{-1}, \ \tilde{c} := (T^{-1})^* c T^{-1} = \tilde{u}^*\tilde{\lambda}\tilde{u}.$$

Since λ has pseudo-differential entries and satisfies (μsc) we have:

$$\tilde{\lambda}_{\alpha\beta} \in \Psi^{\infty}(\mathbb{R}^d), \ \tilde{\lambda}_{\alpha\beta} \in \Psi^{-\infty}(\mathbb{R}^d) \ \text{ for } (\alpha, \beta) \neq (+,+). \tag{7.16}$$

We will check that c satisfies the hypotheses of Thm. 7.1. Since u, u^*, λ preserve $\mathcal{H}(\mathbb{R}^d)\otimes\mathbb{C}^2$ condition (1a) is satisfied. By Remark 7.2, it remains to check condition (2). We compute $\tilde{c}$ and obtain using (7.16) that

$$\tilde{c} = \begin{pmatrix} \tilde{u}^*_{++}\tilde{\lambda}_{++}\tilde{u}_{++} & \tilde{u}^*_{++}\tilde{\lambda}_{++}\tilde{u}_{+-} \\ \tilde{u}^*_{+-}\tilde{\lambda}_{++}\tilde{u}_{++} & \tilde{u}^*_{+-}\tilde{\lambda}_{++}\tilde{u}_{+-} \end{pmatrix} + s,$$

where $s : \mathcal{H}'(\mathbb{R}^d) \otimes \mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2$ is a smoothing operator. Since $\tilde{u}_{+-}, \tilde{u}_{+-} : \mathcal{H}'(\mathbb{R}^d) \to \mathcal{H}(\mathbb{R}^d)$ we have

$$\tilde{c} = \begin{pmatrix} \tilde{u}^*_{++}\tilde{\lambda}_{++}\tilde{u}_{++} & 0 \\ 0 & 0 \end{pmatrix} + s_1,$$

for s_1 as s. Therefore condition (2) is satisfied. $\Box$

Definition 7.7. *We denote by $U_{-\infty}(\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, q)$ the subgroup of $U(\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, q)$ defined by:*

$$U_{-\infty}(\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, q) := \{u \in U(\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, q) \ : \ u - 1\!\!1 \in \Psi^{-\infty}(\mathbb{R}^d) \otimes M_2(\mathbb{C})\}.$$

Corollary 7.8. *The conjugations by elements of $U_{-\infty}(\mathcal{H}(\mathbb{R}^d)\otimes\mathbb{C}^2, q)$ preserve the set of (pure) quasi-free Hadamard states.*

Remark 7.9. *It is easy to see that if $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in U(\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, q)$ and a is invertible, then*

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1\!\!1 & 0 \\ e & 1\!\!1 \end{pmatrix} \begin{pmatrix} g^* & 0 \\ 0 & g^{-1} \end{pmatrix} \begin{pmatrix} 1\!\!1 & f \\ 0 & 1\!\!1 \end{pmatrix} \tag{7.17}$$

for some g invertible and $e^* = -e$, $f^* = -f$. Moreover the matrices

$$(1) \ \begin{pmatrix} 1\!\!1 & 0 \\ e & 1\!\!1 \end{pmatrix}, \ (2) \ \begin{pmatrix} 1\!\!1 & f \\ 0 & 1\!\!1 \end{pmatrix} \ or \ (3) \ \begin{pmatrix} g^* & 0 \\ 0 & g^{-1} \end{pmatrix},$$

where e, $f \in \Psi^{-\infty}(\mathbb{R}^d)$ with $e^* = -e$, $f^* = -f$, and $g - 1\!\!1 \in \Psi^{-\infty}(\mathbb{R}^d)$ with g, g^* invertible, belong to $U_{-\infty}(\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, q)$.

7.4. **Pure Hadamard states.** We now characterize pure Hadamard states with pseudo-differential entries and discuss some examples.

Theorem 7.10. *Let $\lambda \in \Psi^{\infty}(\mathbb{R}^d) \otimes M_2(\mathbb{C})$. Then λ is the two-point function of a pure Hadamard state iff*

$$\begin{array}{rl} \tilde{\lambda}_{++} = & \mathbb{1} + a_{-\infty} a_{-\infty}^*, \\ \tilde{\lambda}_{--} = & a_{-\infty}^* a_{-\infty}, \\ \tilde{\lambda}_{+-} = & \tilde{\lambda}_{-+}^* = a_{-\infty}(\mathbb{1} + a_{-\infty}^* a_{-\infty})^{\frac{1}{2}} \end{array} \tag{7.18}$$

for some $a_{-\infty} \in \Psi^{-\infty}(\mathbb{R}^d)$.

Proof. Set $\tilde{\eta} = 2\tilde{\lambda} - \tilde{q}$. From Prop. 2.6 we see that λ is the two-point function of a pure state iff

$$i)\ \tilde{\eta} \geq 0,\ ii)\ \tilde{\eta}\tilde{q}^{-1}\tilde{\eta} = \tilde{q}. \tag{7.19}$$

Writing $\tilde{\eta}$ as $\begin{pmatrix} a & b \\ b^* & c \end{pmatrix}$ we obtain that (7.19) is equivalent to:

$$\begin{array}{rl} i') & a \geq 0,\ c \geq 0,\ |(u|bv)| \leq (u|au)^{\frac{1}{2}}(v|cv)^{\frac{1}{2}},\ u, v \in \mathcal{H}(\mathbb{R}^d), \\ ii') & a^2 = \mathbb{1} + bb^*,\ c^2 = \mathbb{1} + b^*b,\ ab - bc = 0. \end{array} \tag{7.20}$$

Note that if b is a bounded operator on $L^2(\mathbb{R}^d)$ then:

$$bf(b^*b) = f(bb^*)b, \text{ for any Borel function } f. \tag{7.21}$$

In fact (7.21) is immediate for $f(\lambda) = (\lambda - z)^{-1}$, $z \in \mathbb{C}\backslash\mathbb{R}$ and extends to all Borel functions by a standard argument.

Since $a, c \geq 0$ by *i')*, the first two equations of *ii')* yield

$$a = (\mathbb{1} + bb^*)^{\frac{1}{2}},\ c = (\mathbb{1} + b^*b)^{\frac{1}{2}}.$$

The third equation of *ii')* then holds using (7.21). The second condition in *i')* is equivalent to $\|(\mathbb{1} + bb^*)^{\frac{1}{2}} b (\mathbb{1} + b^*b)^{\frac{1}{2}}\| \leq 1$, which holds using again (7.21).

Going back to $\tilde{\lambda}$ we obtain

$$\tilde{\lambda} = \frac{1}{2}\begin{pmatrix} (\mathbb{1} + bb^*)^{\frac{1}{2}} + \mathbb{1} & b \\ b^* & (\mathbb{1} + b^*b)^{\frac{1}{2}} - \mathbb{1} \end{pmatrix}. \tag{7.22}$$

Let now

$$a := \frac{b}{\sqrt{2}}((\mathbb{1} + b^*b)^{\frac{1}{2}} + \mathbb{1})^{\frac{1}{2}}.$$

Using (7.21) we obtain by an easy computation that

$$\mathbb{1} + a^*a = \frac{1}{2}((\mathbb{1} + b^*b)^{\frac{1}{2}} + \mathbb{1}),\ \mathbb{1} + aa^* = \frac{1}{2}((\mathbb{1} + bb^*)^{\frac{1}{2}} + \mathbb{1}),\ b = 2a(\mathbb{1} + a^*a)^{\frac{1}{2}}.$$

Hence $\tilde{\lambda}$ in (7.22) can be rewritten as:

$$\tilde{\lambda} = \begin{pmatrix} \mathbb{1} + aa^* & a(\mathbb{1} + a^*a)^{\frac{1}{2}} \\ (\mathbb{1} + a^*a)^{\frac{1}{2}} a^* & a^*a \end{pmatrix}. \tag{7.23}$$

By Prop. 7.4 λ satisfies (μsc) iff a^*a, $a(\mathbb{1} + a^*a)^{\frac{1}{2}} \in \Psi^{-\infty}$, which is equivalent to $a \in \Psi^{-\infty}$. $\Box$

Proposition 7.11. *Let $\lambda_i \in \Psi^{\infty}(\mathbb{R}^d) \otimes M_2(\mathbb{C})$, $i = 1, 2$, be two-point functions of pure Hadamard states (for the model Klein-Gordon equation). Then there exists $u \in U_{-\infty}(\mathcal{H}(\mathbb{R}^d) \otimes \mathbb{C}^2, q)$ s.t.*

$$\lambda_2 = u^* \lambda_1 u.$$

Proof. Without loss of generality we can assume that $\tilde\lambda_1 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix}$ and $\tilde\lambda_2$ is given by (7.23) for $a \in \Psi^{-\infty}$. Then

$$\tilde u = \begin{pmatrix} (\mathbb{1}+aa^*)^{\frac12} & a \\ a^* & (\mathbb{1}+a^*a)^{\frac12} \end{pmatrix}$$

belongs to $U_\infty(\mathcal{H}(\mathbb{R}^d)\otimes\mathbb{C}^2, \tilde q)$ and satisfies $\tilde u^*\tilde\lambda_1\tilde u = \tilde\lambda_1$. $\square$

7.4.1. *Canonical Hadamard state.* Once having fixed $r \in \mathcal{M}$, let us consider the two-point function

$$\lambda(r) := \begin{pmatrix} (r+r^*)^{-1} & (r+r^*)^{-1}r \\ r^*(r+r^*)^{-1} & r^*(r+r^*)^{-1}r \end{pmatrix}.$$

An easy computation shows that

$$\tilde\lambda(r) = (T(r)^{-1})^*\lambda(r)T(r)^{-1} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix}.$$

This is a particular case of Theorem 7.10 with $a_{-\infty} = 0$ and it follows that $\lambda(r)$ is the two-point function of a pure Hadamard state. One can show that it is distinguished among all two-point functions $\lambda : \mathcal{H}(\mathbb{R}^d)\otimes\mathbb{C}^2 \to \mathcal{H}(\mathbb{R}^d)\otimes\mathbb{C}^2$ of pure quasi-free states by the property

$$\operatorname{Ran} P_\pm \subset C_\pm(r),$$

where $P_\pm$ is defined on $H^1(\mathbb{R}^d)\oplus L^2(\mathbb{R}^d)$ by

$$P_\pm := \tfrac12\mathbb{1} \pm q\eta, \quad \eta = \lambda - \frac12 q.$$

We now study the dependence of $\lambda(r)$ on $r \in \mathcal{M}$.

Proposition 7.12. *Let:*

$$\mathcal{G} := \{(g,f) \,:\, g-\mathbb{1},\ f \in \Psi^{-\infty}(\mathbb{R}^d),\ g, g^* : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d) \text{ invertible, } f = -f^*\}.$$

We equip $\mathcal{G}$ with the group structure given by:

$$\begin{aligned} &\mathrm{Id} := (\mathbb{1}, 0),\\ &G_2G_1 := (g_2g_1, (g_2^*)^{-1}f_1g_2^{-1} + f_2), \text{ for } G_i = (g_i, f_i). \end{aligned}$$

Then the following holds:

(1) *the map*

$$\mathcal{G} \ni G = (g,f) \mapsto u_G := \begin{pmatrix} g^* & 0 \\ 0 & g^{-1} \end{pmatrix}\begin{pmatrix} \mathbb{1} & f \\ 0 & \mathbb{1} \end{pmatrix} \in U_{-\infty}(\mathcal{H}(\mathbb{R}^d)\otimes\mathbb{C}^2, q)$$

is a group homomorphism.

(2) *$\mathcal{G}$ acts transitively on $\mathcal{M}$ by*

$$\alpha_G(r) := (g^*)^{-1}rg^{-1} + f,\ r \in \mathcal{M},\ G = (g,f) \in \mathcal{G}.$$

Proof. Statement (1) is an easy computation. Let us prove (2).

We first check that α_G preserves $\mathcal{M}$. Let $r \in \mathcal{M}$ and $\tilde r = \alpha_G(r)$ for $G \in \mathcal{G}$. Clearly $\tilde r - r \in \Psi^{-\infty}$ so $\tilde r - (b^*)^{(-1)} = r - (b^*)^{(-1)} + \Psi^{-\infty} \in \Psi^{-\infty}$. It remains to check that

$$\tilde r + \tilde r^* \sim \epsilon^{-1}. \tag{7.24}$$

This is obvious if $G = (\mathbb{1}, f)$, since then $\tilde r = r + f$ and $f^* = -f$.

Assume now that $G = (g, 0)$, so that $\tilde r + \tilde r^* = (g^*)^{-1}(r+r^*)g^{-1}$, and $g - \mathbb{1} \in \Psi^{-\infty}$, $g, g^* : L^2 \to L^2$ invertible. It follows that

$$(\tilde r + \tilde r^*)^{-1} = g(r+r^*)^{-1}g^* = \frac12\epsilon + \Psi^0. \tag{7.25}$$

Since $r \in \mathcal{M}$ we have $r + r^* \sim \epsilon^{-1}$, hence $(r + r^*)^{-1} \sim \epsilon$, by the Kato Heinz inequality. In particular we have $(r + r^*)^{-1} \geq c_0 > 0$. Using then (7.25) we obtain that:

$$\begin{aligned} (\tilde{r} + \tilde{r}^*)^{-1} \geq & \quad c_3 > 0, \\ (\tilde{r} + \tilde{r}^*)^{-1} \geq & \quad \tfrac{1}{2}\epsilon - c_4. \end{aligned}$$

This implies that $(\tilde{r} + \tilde{r}^*)^{-1} \geq c\epsilon$ for some $c > 0$. On the other hand (7.25) directly implies that $(\tilde{r} + \tilde{r}^*)^{-1} \leq c\epsilon$ for some $c > 0$. Therefore we have $(\tilde{r} + \tilde{r}^*)^{-1} \sim \epsilon$, which implies (7.24) by applying Kato-Heinz theorem once again. This completes the proof that α_G preserves $\mathcal{M}$.

It remains to prove that the action is transitive.

let $r_i \in \mathcal{M}$, $i = 1, 2$ As we saw above $(r_i + r_i^*)^{-1} \in \Psi^1$ and $(r_i + r_i^*)^{-1} \sim \epsilon$. By Prop. 4.2 we obtain that $(r_i + r_i^*)^{-\frac{1}{2}} \in \Psi^{\frac{1}{2}}$ and by Kato-Heinz theorem we have $(r_i + r_i^*)^{-\frac{1}{2}} \sim \epsilon^{\frac{1}{2}}$. In particular $(r_i + r_i^*)^{-\frac{1}{2}}$ is bijective from $H^{\frac{1}{2}}(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$. It follows that

$$(r_2 + r_2^*)^{-\frac{1}{2}} = g(r_1 + r_1^*)^{-\frac{1}{2}} = (r_1 + r_1^*)^{-\frac{1}{2}} g^*, \tag{7.26}$$

where g, g^* are invertible on $L^2(\mathbb{R}^d)$. Using also that $r_1 - r_2 \in \Psi^{-\infty}$, we obtain that $g - \mathbb{1} \in \Psi^{-\infty}$. From (7.26) we get:

$$r_2 + r_2^* = (g^*)^{-1}(r_1 + r_1^*)g^{-1}. \tag{7.27}$$

We set now

$$r_2 - r_2^* =: (g^*)^{-1}(r_1 - r_1^*)g^{-1} + 2f. \tag{7.28}$$

Clearly $f^* = -f$, and since $g - \mathbb{1}$ and $r_1 - r_2$ belong to $\Psi^{-\infty}$, we see that $f \in \Psi^{-\infty}$. From (7.27), (7.28) we obtain that $r_2 = (g^*)^{-1} r_1 g^{-1} + f = \alpha_G(r_1)$, for $G = (g, f)$. This completes the proof of the proposition. □

The following theorem explains the dependence of the pure quasi-free state with two-point function $\lambda(r)$ on the choice of $r \in \mathcal{M}$.

Theorem 7.13. *We have*

$$\lambda(\alpha_G(r)) = u_G^* \lambda(r) u_G, \ \forall\ r \in \mathcal{M},\ G \in \mathcal{G}.$$

Proof. writing $\lambda(r)$ as:

$$\lambda(r) = \begin{pmatrix} \mathbb{1} & 0 \\ r^* & \mathbb{1} \end{pmatrix} \begin{pmatrix} (r + r^*)^{-1} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbb{1} & r \\ 0 & \mathbb{1} \end{pmatrix},$$

we easily obtain that if $u = \begin{pmatrix} \mathbb{1} & f \\ 0 & \mathbb{1} \end{pmatrix}$, then

$$u^* \lambda(r) u = \lambda(r + f),$$

and if $u = \begin{pmatrix} g^* & 0 \\ 0 & g^{-1} \end{pmatrix}$, then

$$u^* \lambda(r) u = \lambda((g^*)^{-1} r g^{-1}).$$

This completes the proof of the theorem. □

7.5. **The static case.** Let us illustrate our results in the *static case*, when $a(t, \mathrm{x}, D_{\mathrm{x}})$ is independent on t. We assume for simplicity that $a(\mathrm{x}, D_{\mathrm{x}}) \geq m^2 > 0$, in order to avoid infrared problems. We can work in an abstract setting and denote by $a > 0$ a selfadjoint operator on a (complex) Hilbert space $\mathfrak{h}$. We set $\epsilon := a^{\frac{1}{2}}$.

The solution of the Cauchy problem:

$$\left\{\begin{array}{l} \partial_t^2\phi(t) + a\phi(t) = 0, \\ \phi(0) = f_0, \\ \mathrm{i}^{-1}\partial_t\phi(0) = f_1, \end{array}\right. \tag{7.29}$$

is:

$$\phi(t) = \tfrac{1}{2}\mathrm{e}^{\mathrm{i}t\epsilon}(f_0 + \epsilon^{-1}f_1) + \tfrac{1}{2}\mathrm{e}^{-\mathrm{i}t\epsilon}(f_0 - \epsilon^{-1}f_1) =: U(t,0)f.$$

Therefore, when $\mathfrak{h} = L^2(\mathbb{R}^d)$ and $\epsilon \in \Psi^1(\mathbb{R}^d)$ we can choose

$$b(t) = \epsilon, \; u_\pm(t,s) = \mathrm{e}^{\pm\mathrm{i}(t-s)\epsilon}, \; d_\pm(s) = \frac{1}{2}\mathbb{1}, \; r_\pm(s) = \epsilon^{-1}.$$

Remark 7.14. *Using the reduction to the model case described in Subsect. 5.2, one obtains $a(t, \mathrm{x}, D_{\mathrm{x}})$ independent on t if the metric is static and the electric field vanishes, i.e. $\partial_i V + \partial_t A_i \equiv 0$, $i = 1, \dots, d$.*

For sake of completeness we list below the essential examples of Hadamard states in the static case.

- The two-point function of the vacuum state is:

  $$(f|\lambda_{\mathrm{vac}}f) = \frac{1}{2}(f_0 + \epsilon^{-1}f_1|\epsilon(f_0 + \epsilon^{-1}f_1))_{\mathfrak{h}}.$$

  The matrix elements of $\tilde{\lambda}_{\mathrm{vac}}$ are:

  $$\tilde{\lambda}_{++} = \mathbb{1}, \quad \tilde{\lambda}_{--} = \tilde{\lambda}_{+-} = \tilde{\lambda}_{-+} = 0.$$

  It follows that λ_{vac} equals to $\lambda(\epsilon^{-1})$ with the notation in Subsect. 7.4.1. Setting

  $$\phi_+(t) := U(t,0)P_+f = U(t,0)(q\lambda)f$$

  we have

  $$\phi_+(t) = \tfrac{1}{2}\mathrm{e}^{\mathrm{i}t\epsilon}(f_0 + \epsilon^{-1}f_1).$$

- Let us consider a special case of Theorem 7.5, namely let λ be such that the entries of $\tilde{\lambda}$ are given by

  $$\tilde{\lambda}_{++} = \mathbb{1} + a, \quad \tilde{\lambda}_{+-} = \tilde{\lambda}_{-+}^* = 0, \quad \tilde{\lambda}_{--} = b,$$

  where $a \in \Psi^\infty(\mathbb{R}^d)$ and $b \in \Psi^{-\infty}(\mathbb{R}^d)$ are both assumed to be positive. The corresponding state is not pure unless $a = b = 0$. More explicitly, λ is given by

  $$\lambda = \frac{1}{2}\begin{pmatrix} \epsilon + \epsilon^{\frac{1}{2}}(a+b)\epsilon^{\frac{1}{2}} & \mathbb{1} + \epsilon^{\frac{1}{2}}(a-b)\epsilon^{-\frac{1}{2}} \\ \mathbb{1} + \epsilon^{-\frac{1}{2}}(a-b)\epsilon^{\frac{1}{2}} & \epsilon^{-1} + \epsilon^{-\frac{1}{2}}(a+b)\epsilon^{-\frac{1}{2}} \end{pmatrix}$$

  Defining $\phi_+(t)$ as before we get

  $$\begin{aligned}\phi_+(t) = \; & \tfrac{1}{2}\mathrm{e}^{\mathrm{i}t\epsilon}\left((\mathbb{1} + \epsilon^{-\frac{1}{2}}a\epsilon^{\frac{1}{2}})f_0 + \epsilon^{-1}(\mathbb{1} + \epsilon^{-\frac{1}{2}}a\epsilon^{\frac{1}{2}})f_1\right) \\ & + \tfrac{1}{2}\mathrm{e}^{-\mathrm{i}t\epsilon}\left(\epsilon^{-\frac{1}{2}}b\epsilon^{\frac{1}{2}}f_0 - \epsilon^{-\frac{1}{2}}b\epsilon^{-\frac{1}{2}}f_1\right).\end{aligned}$$

  One can show that the thermal state at inverse temperature β is obtained by taking

  $$a = b = \frac{\mathrm{e}^{-\beta\epsilon}}{\mathbb{1} - \mathrm{e}^{-\beta\epsilon}}.$$

8. Hadamard states on general space-times

8.1. **Space-times with compact Cauchy surfaces.** The results in Sects. 4, 5, 6 and 7 extend verbatim to the case where $\mathbb{R}^d$ is replaced by a compact manifold S. It suffices to replace everywhere $\mathcal{E}(\mathbb{R}^d)$, $\mathcal{H}(\mathbb{R}^d)$ and $\mathcal{D}(\mathbb{R}^d)$ by $\mathcal{D}(S)$ and similarly for their dual spaces. The Weyl pseudo-differential calculus has to be replaced by the standard calculus on compact manifolds. This case is related to the results in [J1, JS]

Remark 8.1. *In* [J1, JS]*, a different convention is employed for the symplectic form acting on Cauchy data. This amounts to considering* $(\phi(s), \partial_t\phi(s))$ *as Cauchy data instead of* $(\phi(s), \mathrm{i}^{-1}\partial_t\phi(s))$*. A two-point function* $\lambda_{\rm Ju}$ *in the convention used in* [J1, JS] *corresponds in our notation to the two point function* $\lambda = v\lambda_{\rm Ju}v^*$*, where* v *is diagonal with entries* $v_{++} = \mathbb{1}$ *and* $v_{--} = \mathrm{i}\mathbb{1}$*.*

In [JS, Thm. 5.10] it is shown how to construct families of operators $J(t) \in C^\infty(\mathbb{R}, \Psi^1(S))$, $R(t) \in C^\infty(\mathbb{R}, \Psi^0(S))$, such that

$$\lambda = \frac{1}{2}\begin{pmatrix} RJ^{-1}R + J & \mathbb{1} - \mathrm{i}RJ^{-1} \\ \mathbb{1} + \mathrm{i}J^{-1}R & J^{-1} \end{pmatrix}$$

is the two-point function of a pure Hadamard state on $\mathbb{R} \times S$. In our approach, this corresponds to setting

$$R(t) = \frac{\mathrm{i}}{2}\left(b(t) - b^*(t)\right), \quad J(t) = \frac{1}{2}\left(b(t) + b^*(t)\right),$$

where $b(t)$ is as in Theorem 6.3. Using $r(t) = b^*(t)^{(-1)} \mod C^\infty(\mathbb{R}, \Psi^{-\infty})$, it is not difficult to check the microlocal spectrum condition by means of Theorem 7.1. It is worth pointing out that one of the advantages of basing the construction on $r(t)$ (as we do) rather than on $b(t)$ is that the former is more closely related to the operator $\epsilon(t)$, cf. Theorem 6.3.

Remark 8.2. *Since* S *is compact we know that* $\mathrm{Op}(a) : H^m(S) \to H^p(S)$ *is Hilbert-Schmidt for any* $m, p \in \mathbb{R}$ *and* $a \in \Psi^{-\infty}(\mathbb{R}^d)$*. By Shale's theorem it follows that the CCR representations obtained from two pure Hadamard states as in Thm. 7.10 are unitarily equivalent, since two such states are obtained from one another by a symplectic transformation in* $U_\infty(\mathcal{D}(S) \otimes \mathbb{C}^2, q)$*.*

8.2. **General space-times.** In this section we give a new construction of quasi-free Hadamard states on an arbitrary globally hyperbolic space-time M.

Before doing so, let us mention that existence of Hadamard states on an arbitrary globally hyperbolic space-time M has already been proved by Fulling, Narcowich and Wald using a deformation argument [FNW]. Roughly speaking, one fixes a Cauchy surface S and defines a deformed space-time M' which overlaps with M on a suitable neighborhood of S, but possesses an ultra-static region in the causal past of S. It is not difficult to construct a Hadamard state in that region, for instance by taking the associated ground state. By the propagation argument of [FSW], this gives a Hadamard state on M', hence in a neighborhood of S, and using the same propagation argument again one obtains a Hadamard state on M. An obvious drawback of this construction is that it is not very explicit and the various distinct states which one can obtain this way are difficult to compare in practice.

In our approach, we reduce the general problem to the special case of space-times considered by us in Sections 5-6 (or simply to the case of a compact Cauchy surface). Namely, using a suitable partition of unity, we glue together Hadamard states on smaller regions of the space-time. Although the procedure does in general not preserve pureness, local properties of the state are under control.

The steps of the construction are the following:

We fix a Cauchy surface S, so that we can assume that $M = \mathbb{R} \times S$ and the metric g is of the form (5.4).

We choose for an open set Ω in M, and $forn \in \mathbb{N}$ open, pre-compact sets U_n, $\tilde{U}_n$ in S, constants $0 < \delta_n$ such that:

$$
(8.1) \qquad \begin{array}{rl}
(i) & U_n \Subset \tilde{U}_n,\ \bigcup_n U_n = S,\\
(ii) & \tilde{U}_n \text{ are coordinate charts for } S,\\
(iii) & y \in \Omega,\ J(y) \cap U_n \neq \emptyset \ \Rightarrow\ y \in]-\delta_n, \delta_n[\times \tilde{U}_n =: \tilde{\Omega}_n,\\
(iv) & \Omega \text{ is a neighborhood of } S \text{ in } M.
\end{array}
$$

In *(iii)* $J(y)$ denotes the causal shadow of $y \in M$. This is clearly possible.

We fix a partition of unity $1 = \sum_n \chi_n^2$ of S, with $\chi_n \in C_0^\infty(U_n)$ for $n \in \mathbb{N}$. Denoting still by χ_n the map $\chi_n \otimes \mathbb{1}$ on $C_0^\infty(S) \otimes \mathbb{C}^2$, we note that

$$
(8.2) \qquad q = \sum_n \chi_n^* q \chi_n.
$$

Fix for each $n \in \mathbb{N}$ a coordinate map $\varphi_n : \tilde{U}_n :\to V_n$, where V_n is a neighborhood of 0 in $\mathbb{R}^d$. The symplectic form σ on $C_0^\infty(\tilde{U}_n) \otimes \mathbb{C}^2$ transported to $C_0^\infty(V_n) \otimes \mathbb{C}^2$ will be given by (5.5).

We also transport with φ_n the Klein-Gordon operator P on $\tilde{\Omega}_n$ to an operator on $]-\delta_n, \delta_n[\times V_n \subset \mathbb{R} \times \mathbb{R}^d$. We can extend this operator to $\mathbb{R} \times \mathbb{R}^d$ so that it satisfies the conditions in Sect. 5. Let us denote by P_n the Klein-Gordon operator on $\mathbb{R} \times \mathbb{R}^d$ obtained in this way. We choose for each $n \in \mathbb{N}$ a two-point function c_n (acting on the space of Cauchy data) of a quasi-free state, which is Hadamard for P_n. We will have in particular

$$
(8.3) \qquad c_n \geq 0,\ c_n \geq q.
$$

We restrict c_n to $C_0^\infty(\tilde{V}_n) \otimes \mathbb{C}^2$ and transport it back to $C_0^\infty(\tilde{U}_n) \otimes \mathbb{C}^2$ by φ_n^{-1}, denoting it by λ_n. Finally we set:

$$
\lambda := \sum_{n \in \mathbb{N}} \chi_n^* \lambda_n \chi_n,
$$

which is well defined as a two-point function on $C_0^\infty(S) \otimes \mathbb{C}^2$, since the sum is locally finite.

Since $q = \sum \chi_n^* q \chi_n$, and c_n was the two-point function of a gauge-invariant quasi-free state, we deduce from (8.3) that $\lambda \geq 0$, $\lambda \geq q$, i.e. λ is the two-point function of a gauge-invariant quasi-free state.

It remains to check that λ satisfies the Hadamard condition, i.e. that

$$
\Lambda = (\rho \circ E)^* \lambda (\rho \circ E)
$$

satisfies (μsc). By the well-known propagation of [FSW](see also [SV2]) that is suffices to check (μsc) in $T^*\Omega \times T^*\Omega \backslash \{0\}$, since Ω is a neighborhood of S in M by (8.1). Set:

$$
\Lambda_n := (\rho \circ E)^* \chi_n^* \lambda_n \chi_n (\rho \circ E),
$$

so that $\Lambda = \sum_n \Lambda_n$. It suffices to check that Λ_n satisfies (μsc) in $T^*\Omega \times T^*\Omega \backslash \{0\}$.

Using the support properties of E and condition (8.1) *(iii)*, we obtain that the restriction to $\Omega \times \Omega$ of the distribution kernel of Λ_n is supported in $\tilde{\Omega}_n \times \tilde{\Omega}_n$. Therefore, up to diffeomorphisms, Λ_n is equal to

$$
C_n := (\rho \circ E_n)^* \chi_n^* \lambda_n \chi_n (\rho \circ E_n)
$$

on $\tilde{\Omega}_n \times \tilde{\Omega}_n$, where E_n is the propagator associated to P_n. Using the invariance of the wavefront set under diffeomorphisms, it follows that Λ_n satisfies the microlocal

spectrum condition. Therefore Λ is the two-point function of a gauge-invariant quasi-free Hadamard state.

Appendix A. Various proofs

A.1. **Proof of Lemma 4.7.** Set $u(t,s) := \mathrm{Texp}(\int_s^t \mathrm{i}\epsilon(\sigma)d\sigma)$. We claim that it suffices to prove that

$$u(t,s)s_{-\infty}(t,s) \in \Psi^{-\infty}(\mathbb{R}^d), \ \forall\ (t,s) \in \mathbb{R}^2. \tag{A.4}$$

In fact we have

$$\begin{aligned}\partial_s u(t,s)s_{-\infty}(t,s) = &\ u(t,s)\left(-\mathrm{i}\epsilon(s)s_{-\infty}(t,s) + \partial_s s_{-\infty}(t,s)\right),\\ \partial_t u(t,s)s_{-\infty}(t,s) = &\ u(t,s)\left(\mathrm{i}u(s,t)\epsilon(t)u(t,s)s_{-\infty}(t,s) + \partial_t s_{-\infty}(t,s)\right).\end{aligned}$$

We note that $-\mathrm{i}\epsilon(s)s_{-\infty}(t,s) + \partial_s s_{-\infty}(t,s) \in \Psi^{-\infty}(\mathbb{R}^d)$, and by Prop. 4.5 (2) $\mathrm{i}u(s,t)\epsilon(t)u(t,s)s_{-\infty}(t,s) + \partial_t s_{-\infty}(t,s) \in \Psi^{-\infty}(\mathbb{R}^d)$. We can argue similarly to control higher derivatives in (t,s).

We first claim that

$$\langle D_x\rangle^m u(t,s)\langle D_x\rangle^{-m} \in B(L^2(\mathbb{R}^d)), \ m \in \mathbb{R}. \tag{A.5}$$

In fact by Prop. 4.5 we know that $u(s,t)\langle D_x\rangle^m u(t,s) \in \Psi^m(\mathbb{R}^d)$ and is moreover elliptic in this class, which proves (A.5).

To prove (A.4) we will use the Beals criterion recalled in the proof of Prop. 4.2, and show that

$$\langle D_x\rangle^m \mathrm{ad}_x^\alpha \mathrm{ad}_{D_x}^\beta (u(t,s)s_{-\infty}(t,s)) \in B(L^2(\mathbb{R}^d)), \ \forall\ \alpha,\beta \in \mathbb{N}^d, \ m \in \mathbb{N}. \tag{A.6}$$

We note that for $i = 1, \dots, d$:

$$\begin{aligned}[D_i, u(t,s)s_{-\infty}] = &\ u(t,s)(u(s,t)D_i u(t,s) - D_i)s_{-\infty} + u(t,s)[D_i, s_{-\infty}],\\ [x_i, u(t,s)s_{-\infty}] = &\ u(t,s)(u(s,t)x_i u(t,s) - x_i)s_{-\infty} + u(t,s)[x_i, s_{-\infty}].\end{aligned}$$

By Prop. 4.5 we know that $u(s,t)D_i u(t,s) - D_i \in \Psi^1(\mathbb{R}^d)$. On the other hand we have:

$$\begin{aligned}u(s,t)x_i u(t,s) - x_i = &\ \mathrm{i}\int_s^t u(s,\sigma)[\epsilon(\sigma), x_i]u(\sigma,s)d\sigma\\ = &\ \int_s^t u(s,\sigma)a_i(\sigma)u(\sigma,s)d\sigma,\end{aligned}$$

where $a_i(\sigma) \in C^\infty(\mathbb{R}, \Psi^0(\mathbb{R}^d))$. Therefore we obtain that

$$\begin{aligned}&\mathrm{ad}_{D_i} u(t,s)s_{-\infty} = u(t,s)s_{-\infty,i},\\ &\mathrm{ad}_{x_i} u(t,s)s_{-\infty} = u(t,s)r_{-\infty,i},\\ &s_{-\infty,i}, \ r_{-\infty,i} \in \Psi^{-\infty}(\mathbb{R}^d).\end{aligned}$$

Using also (A.5), this implies (A.6) by induction. □

A.2. **Proof of Lemma 6.2.** Set $a(t) = a(t, \mathrm{x}, D_{\mathrm{x}})$. Since $a(t)$ is a second order differential operator,we have

$$a(t) = a_2(t) + a_1(t), \ a_i(t) \in C^\infty(\mathbb{R}, \Psi^i_{\mathrm{ph}}), \ a_i(t) = a_i(t)^*, \ i = 1,2 \tag{A.7}$$

and $a_2(t) = \sum_{ij} D_i a^{ij}(t,\mathrm{x})D_j$. From (5.2) we obtain that $a_2(t) \geq c(t)D^2$. Therefore we can find $r_{-\infty,1}(t) = r_{-\infty,1}(t, D_{\mathrm{x}}) \in C^\infty(\mathbb{R}, \Psi^{-\infty})$ such that

$$a_2(t) - r_{-\infty,1}(t) \geq c(t)(D^2 + 1\!\!1). \tag{A.8}$$

The operator $a_2(t) - r_{-\infty,1}(t)$ is elliptic in $C^\infty(\mathbb{R}, \Psi^2_{\mathrm{ph}})$ and strictly positive. By Prop. 4.2, $\epsilon_1(t) := (a_2(t) - r_{-\infty,1}(t))^{\frac{1}{2}} \in C^\infty(\mathbb{R}, \Psi^1_{\mathrm{ph}})$, and $\epsilon_1(t)$ is elliptic in Ψ^1_{ph} with principal symbol $(k_i a^{ij}(t,\mathrm{x})k_j)^{\frac{1}{2}}$. From (A.7) we get

$$a(t) - r_{-\infty,1}(t) = \epsilon_1^2(t) + a_1(t) = \epsilon_1(t)(1\!\!1 + s_{-1}(t))\epsilon_1(t), \tag{A.9}$$

for $s_{-1}(t) = \epsilon_1(t)^{-1}a_1(t)\epsilon_{-1}(t) \in C^\infty(\mathbb{R}, \Psi^1_{\rm ph})$. We fix a cutoff function $\chi \in C^\infty(\mathbb{R})$ with $\chi(s) \equiv 1$ for $|s| \geq 2$, $\chi(s) \equiv 0$ for $|s| \leq 1$. Then

$$
\begin{aligned}
&\chi(R^{-1}|D_{\rm x}|)s_{-1}(t)\chi(R^{-1}|D_{\rm x}|) \in C^\infty(\mathbb{R}, \Psi^1_{\rm ph}),\\
&s_{-1}(t) - \chi(R^{-1}|D_{\rm x}|)s_{-1}(t)\chi(R^{-1}|D_{\rm x}|) \in C^\infty(\mathbb{R}, \Psi^{-\infty}),\\
&\lim_{R\to\infty} \chi(R^{-1}|D_{\rm x}|)s_{-1}(t)\chi(R^{-1}|D_{\rm x}|) = 0 \text{ in } B(L^2(\mathbb{R}^d)),
\end{aligned}
$$

where we used (4.13) in the last statement. This implies that we can find $R = R(t) \gg 1$ such that:

$$
\begin{aligned}
&\chi(R|D_{\rm x}|)s_{-1}(t)\chi(R|D_{\rm x}|) =: \tilde{s}_{-1}(t) \in C^\infty(\mathbb{R}, \Psi^{-1}_{\rm ph}),\\
&s_{-1}(t) - \tilde{s}_{-1}(t) =: \tilde{s}_{-\infty}(t) \in C^\infty(\mathbb{R}, \Psi^{-\infty}),\\
&\mathbb{1} + \tilde{s}_{-1}(t) \geq (1-\delta)\mathbb{1},\ 0 < \delta < 1.
\end{aligned}
$$

It follows that

$$
a(t) - r_{-\infty,1}(t) - \epsilon_1(t)\tilde{s}_{-\infty}(t)\epsilon_1(t) = \epsilon_1(t)(\mathbb{1} + \tilde{s}_{-1}(t))\epsilon_1(t) =: \tilde{a}(t),
$$

where $\tilde{a}(t) \in C^\infty(\mathbb{R}, \Psi^2_{\rm ph})$, $\tilde{a}(t)$ is elliptic in Ψ^2 with principal symbol $k_i a^{ij}(t, {\rm x})k_j$ and strictly positive. We set

$$
\begin{aligned}
r^{\rm w}_{-\infty}(t, {\rm x}, D_{\rm x}) :=&\quad r_{-\infty,1}(t) - \epsilon_1(t)\tilde{s}_{-\infty}(t)\epsilon_1(t) \in C^\infty(\mathbb{R}, \Psi^{-\infty}),\\
\epsilon^{\rm w}(t, {\rm x}, D_{\rm x}) :=&\quad (\tilde{a}(t))^{\frac12} \in C^\infty(\mathbb{R}, \Psi^1_{\rm ph})
\end{aligned}
$$

Again by Prop. 4.2 $\epsilon^{\rm w}(t, {\rm x}, D_{\rm x})$ has principal symbol $(k_i a^{ij}(t, {\rm x})k_j)^{\frac12}$. This completes the construction of $\epsilon(t)$ and $r_{-\infty}(t)$. The uniqueness modulo $\Psi^{-\infty}$ follows from the fact that $\epsilon^{\rm w}(t, {\rm x}, D_{\rm x}) = a(t, {\rm x}, D_{\rm x})^{\frac12}$, hence the asymptotic expansion of its symbol is unique. □

A.3. **Proof of Thm. 6.3.** We start by proving an auxiliary lemma.

Lemma A.1. *Let $F : C^\infty(\mathbb{R}, \Psi^\infty(\mathbb{R}^d)) \to C^\infty(\mathbb{R}, \Psi^\infty(\mathbb{R}^d))$ a map such that:*

$$
F : C^\infty(\mathbb{R}, \Psi^0_{\rm (ph)}(\mathbb{R}^d)) \to C^\infty(\mathbb{R}, \Psi^{-1}_{\rm (ph)}(\mathbb{R}^d)), \tag{A.10}
$$

$$
b_1 - b_2 \in C^\infty(\mathbb{R}, \Psi^{-j}_{\rm (ph)}(\mathbb{R}^d)) \ \Rightarrow\ F(b_1) - F(b_2) \in C^\infty(\mathbb{R}, \Psi^{-j-1}_{\rm (ph)}(\mathbb{R}^d)),\ \forall\ j \in \mathbb{N}. \tag{A.11}
$$

Let also $a \in C^\infty(\mathbb{R}, \Psi^0_{\rm (ph)}(\mathbb{R}^d))$. Then there exists a solution $b \in C^\infty(\mathbb{R}, \Psi^0_{\rm (ph)}(\mathbb{R}^d))$, unique modulo $C^\infty(\mathbb{R}, \Psi^{-\infty}(\mathbb{R}^d))$ of the equation:

$$
b = a + F(b) \ \mathit{mod}\ C^\infty(\mathbb{R}, \Psi^{-\infty}(\mathbb{R}^d)). \tag{A.12}
$$

Proof. We first prove existence. Set $b_0 = a$, $b_n = a + F(b_{n-1})$, $n \geq 1$. Using (A.11) we easily obtain by induction on n that:

$$
b_n - b_{n-1} \in C^\infty(\mathbb{R}, \Psi^{-n}),\ n \geq 1. \tag{A.13}
$$

It follows that we can find $b \in C^\infty(\mathbb{R}, \Psi^0)$ such that $b - b_n \in C^\infty(\mathbb{R}, \Psi^{-n})$, $\forall\ n \in \mathbb{N}$. In fact it suffices to choose

$$
b \sim \sum_{n=0}^{\infty}(b_n - b_{n-1}).
$$

Then

$$
b - a - F(b) = b - b_n + F(b_{n-1}) - F(b) \in C^\infty(\mathbb{R}, \Psi^{-n}),
$$

using (A.11) and the fact that $b - b_n \in C^\infty(\mathbb{R}, \Psi^{-n})$, $b - b_{n-1} \in C^\infty(\mathbb{R}, \Psi^{-n+1})$.

Let us now prove uniqueness. If b, $\tilde{b}$ solve (A.12), then

$$
b - \tilde{b} = F(b) - F(\tilde{b}) \text{ mod } C^\infty(\mathbb{R}, \Psi^{-\infty}),
$$

hence $b-\tilde{b}\in C^\infty(\mathbb{R},\Psi^{-1})$. By induction using (A.11), we obtain that $b-\tilde{b}\in C^\infty(\mathbb{R},\Psi^{-n})$, $\forall\, n\in\mathbb{N}$. The poly-homogeneous case is treated similarly. □

We now prove Thm. 6.3. The proof is divided in several steps.

Step 1: we first determine the operator $b(t)$, modulo $C^\infty(\mathbb{R},\Psi^{-\infty})$. Set $u(t,s)=\mathrm{Texp}(\mathrm{i}\int_s^t b(\sigma)d\sigma)$, for $b(t)\in C^\infty(\mathbb{R},\Psi^1)$, $b(t)$ elliptic in Ψ^1 and $b(t)-b^*(t)\in\Psi^0$. We have:

$$\partial_t u(t,s)=\mathrm{i}b(t)u(t,s),\ \ \partial_t^2 u(t,s)=-b^2(t)u(t,s)+\mathrm{i}\partial_t b(t)u(t,s).$$

By Lemma 6.2 we have

$$(\partial_t^2+a(t))u(t,s)=(\epsilon^2(t)-b^2(t)+\mathrm{i}\partial_t b(t)+r_{-\infty}(t))u(t,s),$$

with $r_{-\infty}(t)\in C^\infty(\mathbb{R},\Psi^{-\infty})$.

Let us try to solve the equation

$$b^2-\epsilon^2=\mathrm{i}\partial_t b \bmod C^\infty(\mathbb{R},\Psi^{-\infty}). \tag{A.14}$$

We look for a solution of (A.14) of the form:

$$b=\epsilon+b_0,\ \ b_0\in C^\infty(\mathbb{R},\Psi^0).$$

Since

$$b^2-\epsilon^2=(\epsilon b_0+b_0\epsilon)+b_0^2=(2\epsilon b_0+[b_0,\epsilon])+b_0^2,$$

we obtain that (A.14) is equivalent to

$$\begin{aligned} b_0= &\ \ (2\epsilon)^{-1}\mathrm{i}\partial_t\epsilon+(2\epsilon)^{-1}\left([\epsilon,b_0]+\mathrm{i}\partial_t b_0-b_0^2\right) \bmod C^\infty(\mathbb{R},\Psi^{-\infty})\\ =: &\ \ (2\epsilon)^{-1}\mathrm{i}\partial_t\epsilon+F(b_0) \bmod C^\infty(\mathbb{R},\Psi^{-\infty}).\end{aligned}\tag{A.15}$$

To solve (A.15) we apply Lemma A.1. Clearly $(2\epsilon)^{-1}\mathrm{i}\partial_t\epsilon\in C^\infty(\mathbb{R},\Psi^0)$ and F maps $C^\infty(\mathbb{R},\Psi^0)$ into $C^\infty(\mathbb{R},\Psi^{-1})$. Since

$$\begin{aligned} & F(b_1)-F(b_2)\\ = &\ (2\epsilon)^{-1}\left([\epsilon,b_1-b_2]+\mathrm{i}\partial_t(b_1-b_2)-(b_1^2-b_2^2)\right)\\ = &\ (2\epsilon)^{-1}\left([\epsilon,b_1-b_2]+\mathrm{i}\partial_t(b_1-b_2)-(b_1-b_2)b_1-b_2(b_1-b_2)\right),\end{aligned}$$

we see that hypothesis (A.11) also holds. Therefore we can find a solution to (A.14) with:

$$b(t)=\epsilon(t)+(2\epsilon)^{-1}\mathrm{i}\partial_t\epsilon \bmod C^\infty(\mathbb{R},\Psi^{-1}). \tag{A.16}$$

This proves condition *(i)* of the theorem.

Note also that if b a solution of (A.14), then $-b^*$ also solves (A.14), since $\epsilon=\epsilon^*$. Therefore if

$$b_+(t)=b(t),\ \ b_-(t)=-b^*(t),\ \text{and}\ u_\pm(t,s)=\mathrm{Texp}(\mathrm{i}\int_s^t b_\pm(\sigma)d\sigma),$$

we have

$$(\partial_t^2+a(t,\mathrm{x},D_{\mathrm{x}}))u_\pm(t,s)=r_{-\infty,\pm}(t)u_\pm(t,s),\ \ r_{-\infty,\pm}(t)\in C^\infty(\mathbb{R},\Psi^{-\infty}).$$

Step 2:

we now solve, modulo smoothing errors, the Cauchy problem (5.3). For $f\in\mathcal{H}'(\mathbb{R}^d)\otimes\mathbb{C}^2$, we look for approximate solutions of (5.3) of the form:

$$u_+(t,s)\left(d_+(s)f_0+n_+(s)f_1\right)+u_-(t,s)\left(d_-(s)f_0+n_-(s)f_1\right). \tag{A.17}$$

We obtain the conditions:

$$\left\{\begin{array}{l} d_+(s)+d_-(s)=\mathbb{1},\\ b_+(s)d_+(s)+b_-(s)d_-(s)=0,\\ n_+(s)+n_-(s)=0,\\ b_+(s)n_+(s)+b_-(s)n_-(s)=\mathbb{1}.\end{array}\right.\tag{A.18}$$

We deduce from (A.16) that $b_\pm$ are elliptic in Ψ^1, $b_\pm = \pm\epsilon + \Psi^0$ and $b_\pm^{(-1)} b_\mp = -\mathbb{1} + \Psi^{-1}$. Therefore the solutions of (A.18) mod $\Psi^{-\infty}$ are given by:

$$\text{(A.19)}\qquad \begin{cases} d_+(s) = & (\mathbb{1} - b_-(s)^{(-1)} b_+(s))^{(-1)},\\ d_-(s) = & (\mathbb{1} - b_+(s)^{(-1)} b_-(s))^{(-1)},\\ n_+(s) = & (b_+(s) - b_-(s))^{(-1)},\\ n_-(s) = & -n_+(s). \end{cases}$$

Note that it follows from (A.19) that:

$$\text{(A.20)}\qquad d_+(s)^{(-1)} n_+(s) = b_-(s)^{(-1)},\ -d_-(s)^{(-1)} n_-(s) = b_+(s)^{(-1)} \text{ mod } \Psi^{-\infty}.$$

Therefore we can rewrite (A.17) as

$$\text{(A.21)}\qquad U(t,s)f := u_+(t,s) d_+(s)\left(f_0 + r_+(s) f_1\right) + u_-(t,s) d_-(s)\left(f_0 - r_-(s) f_1\right),$$

for

$$\text{(A.22)}\qquad r_+(s) = -b_-(s)^{(-1)},\ r_-(s) = b_+(s)^{(-1)} \text{ mod } \Psi^{-\infty}.$$

Since $b_+(s) = b(s)$, $b_-(s) = -b^*(s)$ if we choose:

$$\text{(A.23)}\qquad r(s) = b^*(s)^{(-1)} \text{ mod } \Psi^{-\infty},$$

and fix

$$r_+(s) := r(s),\ r_-(t) := r^*(s),$$

then (A.22) is satisfied. We now check that we can find $r(s)$ satisfying (A.23) such that conditions *(iii)* and *(iv)* in the theorem are satisfied.

Let us denote $b(s)$, $r(s)$, $\epsilon(s)$ simply by b, r, ϵ. Since $b = \epsilon + \Psi^0$ we have $r = \epsilon^{-1} + \Psi^{-2}$, hence *(iii)* is satisfied. Moreover since $\epsilon^{-\frac{1}{2}} \in \Psi^{-\frac{1}{2}}$ by Prop. 4.2, we have

$$r + r^* = 2\epsilon^{-1} + \Psi^{-2} = \epsilon^{-\frac{1}{2}}(2\mathbb{1} + s_{-1}^{\mathrm{w}}(\mathrm{x}, D_{\mathrm{x}}))\epsilon^{-\frac{1}{2}},$$

where $s_{-1}(\mathrm{x},k) \in S^{-1}_{\mathrm{ph}}(\mathbb{R}^{2d})$. We write

$$\begin{aligned} s_{-1}(\mathrm{x},k) = &\ s_{-1}(\mathrm{x},k)\chi(R^{-1}|k| \geq 1) + s_{-1}(\mathrm{x},k)\chi(R^{-1}|k| \leq 1)\\ =: &\ s_{-1,R}(\mathrm{x},k) + s_{-\infty,R}(\mathrm{x},k). \end{aligned}$$

Note that $s_{-\infty,R} \in S^{-\infty}(\mathbb{R}^{2d})$ and $s_{-1,R}$ tends to 0 in $S^0(\mathbb{R}^{2d})$ when $R \to +\infty$. By (4.13) it follows that $2\mathbb{1} + s_{-1,R}^{\mathrm{w}}(\mathrm{x}, D_{\mathrm{x}}) \sim \mathbb{1}$ for R large enough. Therefore replacing r by

$$\tilde{r} = r - \frac{1}{2}\epsilon^{-\frac{1}{2}} s_{-\infty,R}^{\mathrm{w}}(\mathrm{x}, D_{\mathrm{x}})\epsilon^{-\frac{1}{2}} = r + \Psi^{-\infty},$$

we can ensure *(iv)*, keeping (A.23) satisfied.

Collecting what we have done so far we have:

$$\begin{cases} & (\partial_t^2 + a(t,\mathrm{x},D_{\mathrm{x}}))U(t,s)f = r_{-\infty,+}(t) u_+(t,s) d_+(s)(f_0 + r_+(s) f_1)\\ + & r_{-\infty,-}(t) u_-(t,s) d_-(s)(f_0 - r_-(s) f_1),\\ & U(s,s)f = f_0 + t_{-\infty,0}(s) f,\\ & \mathrm{i}^{-1}\partial_t U(s,s) f = f_1 + t_{-\infty,1}(s) f, \end{cases}$$

where $r_{-\infty,\pm}$ and $t_{-\infty,i}$ belong to $C^\infty(\mathbb{R}, \Psi^{-\infty})$. Applying also Lemma 4.7 to the operators $r_{-\infty,\pm}(t) u_\pm(t,s)$, we obtain statement (1) of the theorem.

Finally $\tilde{\phi}(t) = U(t,s)f$ solves

$$\begin{cases} \partial_t^2 \tilde{\phi}(t) + a(t,\mathrm{x},D_{\mathrm{x}})\tilde{\phi}(t) \in C^\infty(\mathbb{R}, \mathcal{H}(\mathbb{R}^d)),\\ \phi(s) - f_0 \in \mathcal{H}(\mathbb{R}^d),\\ \mathrm{i}^{-1}\partial_t \phi(s) - f_1 \in \mathcal{H}(\mathbb{R}^d). \end{cases}$$

By the uniqueness of the Cauchy problem (5.3) we obtain that $\phi(t) - \tilde{\phi}(t) \in C^\infty(\mathbb{R}, \mathcal{H}(\mathbb{R}^d))$, which proves (2).

This completes the proof of the theorem. □

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